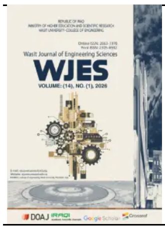

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Review Article

Artificial Intelligence-Based Inverse Design of Plasmonic Structures: A Comparative Review of Conventional and Data-Driven Methods

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ABSTRACT

This study reviews traditional simulation-based methods and artificial intelligence (AI) approaches for the inverse design of plasmonic structures. Conventional techniques such as the Finite Element Method (FEM), Finite-Difference Time-Domain (FDTD), and Beam Propagation Method (BPM) provide accurate electromagnetic predictions but are computationally demanding, especially in large multi-dimensional design spaces. AI-driven approaches, including machine learning, deep learning, and generative models like Generative Adversarial Networks (GANs) and Conditional Tabular GANs (CTGANs), offer faster predictions of structural parameters from optical targets and enable synthetic dataset generation to address data scarcity. The analysis outlines the strengths and limitations of both strategies, emphasizing their complementary role in advancing high-performance plasmonic devices. Particular focus is placed on their importance for sixth-generation (6G) communication systems, which require high-speed, energy-efficient, and densely integrated optical hardware

Keywords: Plasmonics, Inverse Design, Artificial Intelligence (AI), Generative Models CTGAN, 6G Communications

1. Introduction

Plasmonics, a branch of nanophotonics, explores the interaction between electromagnetic waves and free electrons at metal–dielectric interfaces, leading to surface plasmon polaritons (SPPs). These modes confine light beyond the diffraction limit, enabling subwavelength optical manipulation and paving the way for compact photonic components [1]. Consequently, plasmonic structures are central to photonic integrated circuits (PICs), biosensors, quantum communication, and ultrafast computing [2]. Among them, plasmonic logic devices flip-flops, multiplexers, switches, modulators, and logic gates are critical for nanoscale signal processing. They are expected to support sixth-generation (6G) networks that demand high speed, energy efficiency, and dense integration to meet extreme data rates and low latency [3]. Designing efficient plasmonic devices requires precise control of geometry and material properties, as minor variations in waveguide width, gap, or refractive index strongly affect transmission, contrast ratio, and insertion loss [4]. Traditionally, optimization has relied on full-wave electromagnetic simulations such as finite element (FEM), finite-difference time-domain (FDTD), and beam propagation methods (BPM). While accurate, these approaches are computationally costly and impractical for exploring large design spaces with many parameters [5]. To address these challenges, artificial intelligence (AI) has emerged as an effective alternative for accelerating inverse design. Inverse design focuses on identifying structural configurations that yield desired optical responses. AI techniques including machine learning (ML), deep learning (DL), and generative models enable rapid prediction of design parameters and efficient exploration of high-dimensional spaces [6]. Methods based on supervised learning (e.g., Random Forest, Support Vector Regression), deep neural networks (DNNs), and generative adversarial networks (GANs) have demonstrated significant accuracy in determining optimal geometries of plasmonic devices [7]. Fig.1 illustrates the AI-driven workflow: synthetic datasets generated via advanced models capture broad geometric and material variations; learning algorithms map optical targets to structural parameters; and optimized designs are produced with high precision in far less time than traditional simulations.

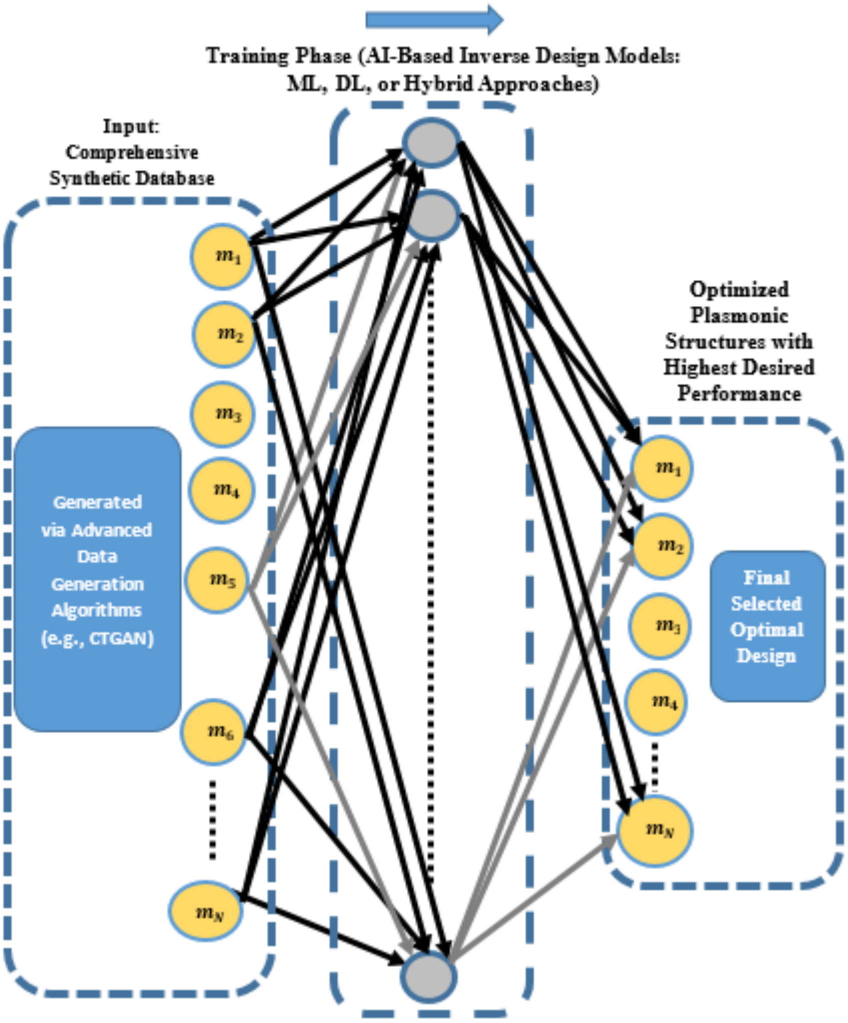

Figure 1. Schematic Representation of The AI-Based Inverse Design Workflow for Plasmonic Structures.

2. Methodology

This comparative review follows a structured and transparent methodology to ensure consistency, reproducibility, and credibility in analyzing the literature on artificial-intelligence-based inverse design of plasmonic structures. The process was designed to comprehensively capture, classify, and evaluate relevant studies published between 2015 and 2025.

2.1 Database Sources

A multi-database search strategy was adopted to ensure broad coverage of high-quality peer-reviewed publications. The databases consulted include IEEE Xplore, Science Direct, Springer Link, Wiley Online Library, and MDPI. These sources collectively cover the leading journals and conferences in photonics, plasmonics, and artificial intelligence.

2.2 Search Strings and Inclusion Criteria

The literature search was conducted using the following main search strings combined with Boolean operators (AND/OR):
“inverse design + plasmonic, AI-based nanophotonics design, machine learning plasmonic waveguide, CTGAN plasmonic, deep learning metasurface.
To ensure scientific relevance, studies were included based on the following criteria:
Peer-reviewed articles or conference proceedings, Explicit implementation of AI or optimization algorithms in plasmonic or nanophotonic design, Quantitative evaluation using metrics such as mean absolute error (MAE), R^2 score, contrast ratio, insertion loss, or modulation depth.

2.3 Review Process Flow

The review followed five systematic stages:
Literature Retrieval: collecting studies from the selected databases using the search strings above.
Screening: filtering duplicates and irrelevant papers through title and abstract review.
Classification: grouping studies based on their design approach: conventional (FEM/FDTD/BPM) or AI-based (ML/DL/CTGAN/VAE).
Quantitative Benchmarking: extracting and comparing key parameters such as dataset size, design variables, and performance metrics.
Synthesis and Discussion: evaluating trends, strengths, and limitations to identify future research opportunities.

2.4 Limitations of the Review

Despite following a systematic methodology, several limitations remain. Only English-language publications were considered, potentially omitting relevant studies in other languages. Variations in datasets, metrics, and reporting standards across studies limit direct quantitative comparability. The review focuses on inverse design using AI; purely theoretical works on plasmonic fundamentals were excluded. Fabrication-level validation remains limited in the literature, which constrains the benchmarking of AI-generated designs against experimentally realized structures.

3. Background and Theoretical Foundations

3.1. Plasmonic Structures: Fundamentals and Applications

Surface plasmon polaritons (SPPs) are tightly confined electromagnetic waves that propagate along the interface between a dielectric and a metal, resulting from the coupling between photons and collective oscillations of free electrons in the metal. These waves exhibit subwavelength confinement and decay exponentially perpendicular to the interface. The behavior of SPPs is governed by classical Maxwell’s equations, along with specific boundary conditions at the metal-dielectric interface [8]. The fundamental dispersion relation that characterizes SPPs at a planar metal-dielectric interface is given by:

$$k_{spp} = \sqrt{\frac{\varepsilon_m \varepsilon_d}{\varepsilon_m + \varepsilon_d}}\, k_\circ \tag{1}$$

where k_{spp} is the propagation constant of the surface plasmon, $k_\circ$ is the free-space wave vector, and $\varepsilon_m, \varepsilon_d$ are the complex permittivities of the metal and dielectric, respectively [9]. This relation shows that $k_{spp} > k_\circ$, meaning SPPs cannot be excited by direct incidence of light from free space and require special coupling techniques (e.g., prism or grating coupling) to match the momentum a requirement known as the phase-matching condition. Moreover, due to the complex nature of the permittivity of metals, the propagation length of SPPs is limited by ohmic losses, which can be described by an exponential decay:

$$L_{SPP} = \frac{1}{Im(k_{spp}).2} \tag{2}$$

To mitigate the trade-off between confinement and loss, hybrid plasmonic waveguides (HPWGs) integrate metal and dielectric layers in engineered geometries to balance field localization with propagation efficiency [10]. These structures underpin diverse nanophotonic devices:

- Waveguides: Achieve extreme subwavelength confinement, enabling dense photonic integration [11].
- Logic Gates and Flip-Flops: Constructed through interference effects, plasmonic gates (AND, OR, NAND) and flip-flops (D-type, SR-latch) have been realized using resonators and nonlinearities [12], [13].
- Switches and Modulators: SPP transmission can be tuned via thermo-optic, electro-optic, or Kerr effects for high-speed switching [14].
- Resonators: Nanoring and nanodisk designs enable narrowband filtering, wavelength selection, and memory [15].
- Multiplexers/Demultiplexers: Key to wavelength-division multiplexing, plasmonic devices enable nanoscale multi-channel routing for future 6G systems [16].

These applications highlight the potential of plasmonics for compact, high-speed, and low-power devices. Given the complexity of geometry–material interactions, AI-driven inverse design has become essential for optimizing next-generation 6G-ready structures.

3.2. Conventional Simulation Techniques

The design and analysis of plasmonic structures have traditionally relied on physics-based numerical simulation techniques that solve Maxwell's equations under appropriate boundary conditions. The most popular among such approaches are the Finite Element Method (FEM), Finite-Difference Time-Domain (FDTD), and the Beam Propagation Method (BPM). In large measure, they have been responsible for investigating and confirming several of the plasmonic phenomena, mostly in geometries where it is not possible to find an analytical solution because of geometry complexity or the presence of multiple layers.

3.2.1 Finite Element Method (FEM)

The Finite Element Method (FEM) works through the discretization of the computational domain into a mesh of fine elements and solving Maxwell's equations within the frequency domain using variational formulations. It is extremely effective for problems dealing with complex geometries and material inhomogeneities and therefore ideal for investigation of hybrid plasmonic waveguide and resonator structures [17]. FEM-based simulation suites like COMSOL Multiphysics and CST Microwave Studio offer very high accuracy and flexibility. Nonetheless, these simulations often demand significant computational resources, particularly when applied to three-dimensional models or extensive parameter sweeps involving multiple design variables.

3.2.2 Finite-Difference Time-Domain (FDTD)

The FDTD method solves Maxwell's curl equations in the time domain by discretizing both space and time using Yee's grid. FDTD is one of the most popular methods in nanophotonics due to its ability to simulate broadband responses in a single run and handle nonlinear and time-dependent effects [18]. It has been extensively applied to study field enhancement in plasmonic nanostructures, SPP propagation, and resonance behavior. Nonetheless, FDTD requires fine meshing around metallic interfaces to capture field discontinuities accurately, often leading to large memory and time requirements.

3.2.3 Beam Propagation Method (BPM)

The Beam Propagation Method is a paraxial approximation technique primarily used to model waveguide propagation in dielectric structures. While it is less suitable for full-wave plasmonic modeling due to the breakdown of the paraxial assumption in metal-dielectric interfaces, BPM has found niche applications in simulating low-loss hybrid plasmonic configurations with small perturbations [19]. Each of these methods has its respective strengths and drawbacks Table 1 [20]. FEM offers superior geometric flexibility, FDTD provides broadband time-domain analysis, and BPM offers fast simulation in paraxial regimes. However, they all share a significant limitation: high computational cost for large parameter sweeps, slow convergence in optimization loops, and limited scalability when dealing with multi-objective inverse design problems. The brute-force nature of parameter tuning in traditional workflows often makes them impractical for real-time or large-scale optimization

Table 1. Comparison of Electromagnetic Simulation Methods in Plasmonics

Method	Strengths	Limitations
FEM (Finite Element Method)	Handles complex geometries Good for material inhomogeneity High accuracy	High computational cost Slow for 3D parameter sweeps Manual tuning time-consuming
FDTD (Finite-Difference Time-Domain)	Broadband simulation in single run Suitable for nonlinear/time-domain effects Widely used in nanophotonics	Requires very fine mesh High memory/time use Slower in large designs
BPM (Beam Propagation Method)	Fast simulation Useful in weakly guiding dielectrics Simple to implement	Not suitable for metals Inaccurate for strong confinement Paraxial approximation fails in plasmonics

3.3 Inverse Design: Definition and Motivation

In photonic and plasmonic engineering, inverse design is the computational process of determining structural or material parameters that yield a desired optical performance. Unlike forward design, which proposes a structure and then analyzes its properties, inverse design begins with performance targets such as transmission, extinction ratio, contrast ratio, or bandwidth and automatically infers the optimal configuration [21]. Plasmonic devices, particularly those using hybrid waveguides or multi-resonator systems, exhibit complex electromagnetic interactions with nonlinear dependencies between geometry and optical response. As design parameters increase (waveguide width, resonator spacing, refractive index, thickness, coupling gaps), brute-force sweeps become impractical, requiring thousands of costly simulations to achieve a target performance [22]. Inverse design overcomes these limitations by framing the task as optimization or regression, where algorithms map performance metrics to structural parameters. This reduces design time, enables discovery of non-intuitive geometries, and expands the solution space beyond manual trial-and-error [23]. Various techniques have been applied to plasmonic structures. For instance, [24] used FDTD-based topology optimization for field confinement, while [25] applied machine learning to accelerate device prediction and retrieval. In [26], neural networks were used for waveguide-cavity spectral design, cutting simulation time significantly. Deep learning optimized plasmonic nanoantennas for tailored scattering [27], topology optimization enhanced nanoaperture trapping efficiency [28], and ML models refined designs for improved contrast ratio, insertion loss, and modulation depth [29]. These advances demonstrate inverse design's versatility in:

- Logic circuits and switches based on engineered transmission and contrast.
- Resonator components such as filters, multiplexers, and nanoantennas requiring precise resonance control.
- Nanoapertures and beam devices for light manipulation, optical trapping, and power distribution.By shifting from trial-and-error to performance-driven optimization, inverse design enhances efficiency, scalability, and fabrication readiness. With artificial intelligence (AI), inverse design has gained greater efficiency. Machine learning (ML) methods including deep neural networks, random forests, and generative models such as GANs can approximate complex nonlinear mappings that are analytically difficult. This enables data-driven, generalizable, and tunable design compatible with experimental and synthetic datasets [30]. Thus, AI serves as the key enabler for rapid, scalable inverse design of next-generation plasmonic devices.

3.4 AI-Based Inverse Design Techniques

The integration of artificial intelligence (AI) into nanophotonics has transformed inverse design by enabling direct inference of optimal geometries from performance targets, in contrast to traditional forward simulations. Several machine learning (ML) techniques have been widely applied**.** Random Forest Regressors (RFRs) are robust and generalizable, even with noisy datasets [31], while Multilayer Perceptrons (MLPs) effectively capture nonlinear relations between structural and optical properties [32]. More recently, Generative Adversarial Networks (GANs) and Conditional Tabular GANs (CTGANs) have been used not only for inverse prediction but also for dataset augmentation, helping to overcome the scarcity of simulation-derived data [33], [34]. Data quality remains critical, as most datasets originate from costly FEM or FDTD solvers. GAN-based augmentation, particularly CTGAN, addresses this by generating diverse, balanced synthetic data that preserves inter-feature correlations [35]. Recent studies validate these approaches: [36] applied deep learning to predict resonance in plasmonic ring resonators, while [37] designed ultra-compact MIM waveguides that outperformed conventional methods. Overall, AI-driven inverse design shortens optimization cycles from days to minutes, improves metrics such as contrast ratio and insertion loss, and enhances fabrication tolerance, representing a paradigm shift toward scalable, real-time, and fabrication-ready nanophotonic design.

3.5 Comparison Between AI-Based and Traditional Design Workflows

Plasmonic device design requires accurate mapping between structural parameters and performance metrics such as contrast ratio, insertion loss, and transmission. Traditionally, this has relied on iterative simulations using FEM, FDTD, or BPM. While accurate, these methods are computationally costly, time-intensive, and dependent on expert supervision. Their limitations include long runtimes, high hardware demand, manual intervention, and restricted exploration of parameter spaces, often leading to suboptimal designs [38]. AI-driven inverse design offers a scalable alternative [39]. Once trained, AI models predict optimal parameters in milliseconds, reducing design cycles from days to minutes. They generalize across high-dimensional spaces, uncover non-intuitive structure performance relationships, and automate optimization. Synthetic data generation with models such as CTGAN further expands datasets without extra simulation cost [40]. Comparative studies confirm these advantages: [41] reported a 93% reduction in design time for a plasmonic switch using deep learning, and [42] achieved higher throughput and lower loss in AI-designed optical splitters. GAN-based augmentation has also enhanced scalability [43]. Hybrid approaches, combining AI with simulation for validation, balance accuracy and efficiency and are increasingly applied in research and industry [44].

3.5.1 Supervised Machine Learning Models

Supervised machine learning (ML) algorithms are powerful tools for inverse design of plasmonic nanostructures, enabling prediction of structural configurations directly from desired optical metrics such as contrast ratio, insertion loss, modulation depth, and transmission. By learning functional mappings between input–output data pairs, these models provide rapid predictions that replace lengthy simulation cycles. Widely applied supervised methods include Random Forest (RF), Support Vector Regression (SVR), Extreme Gradient Boosting (XGBoost), and Light Gradient Boosting Machine (LightGBM).

- Random Forest (RF): An ensemble of decision trees trained on random subsets, robust against overfitting and effective in modeling nonlinear dependencies between optical and structural parameters in hybrid plasmonic waveguides [45].

- Support Vector Regression (SVR): Achieves high accuracy for small to medium datasets but is less scalable and slower than ensemble methods [46].
- XGBoost: A gradient boosting framework that builds successive trees to minimize residual errors, effective for sparse or incomplete datasets and capturing higher-order interactions [47].
- LightGBM: An efficient gradient boosting implementation using histogram-based learning, achieving performance comparable to XGBoost with faster training and lower memory use, ideal for large-scale design tasks [48].

When trained on high-quality datasets whether simulation-based or synthetically generated these models have achieved structural prediction errors below 1 nm, validating their potential for near real-time inverse design in nanophotonics [49], [50]. Moreover, tree-based models offer interpretability through feature importance analysis, providing insights into the influence of optical metrics on structural parameters and supporting deeper physical understanding.

3.5.2 Deep Learning Architectures

Deep learning has emerged as a transformative paradigm in the field of inverse design for plasmonic nanostructures, particularly for addressing high-dimensional, nonlinear design spaces that challenge traditional simulation and regression methods. Unlike shallow machine learning models, deep learning architectures such as Multilayer Perceptrons (MLPs)**,** Convolutional Neural Networks (CNNs), and other advanced neural architectures offer the ability to learn complex mappings between optical performance metrics and design parameters with high fidelity.

3.5.2.1 Multilayer Perceptron (MLPs)

MLPs are fully connected feedforward neural networks consisting of multiple hidden layers with nonlinear activation functions. They are widely used in the inverse design of photonic and plasmonic devices due to their flexibility in modeling complex, non-intuitive relationships between input features (e.g., contrast ratio, insertion loss) and target outputs (e.g., waveguide dimensions, resonator geometries). When trained on normalized and sufficiently large datasets, MLPs can achieve sub-nanometer prediction accuracy for geometrical parameters [51], [52]. However, MLPs typically require careful hyperparameter tuning and benefit significantly from data preprocessing techniques such as feature scaling and dimensionality reduction.

3.5.2.2 Convolutional Neural Networks (CNNs)

Originally designed for image processing, Convolutional Neural Networks (CNNs) have been adapted to inverse problems in nanophotonics by encoding structures as spatial grids or matrices. For instance, photonic crystals and metasurfaces can be represented as pixelated images, allowing CNNs to extract spatial features and learn structure–function mappings [53]. Their hierarchical design makes them effective for capturing multi-scale dependencies, particularly in topology optimization. Deep models, however, require large datasets to avoid overfitting, and generating these through FEM or FDTD simulations is computationally expensive. To overcome this, synthetic data generation using models such as Conditional GANs (cGANs) augments training sets without incurring high simulation costs [54], [55]. Once trained, CNNs predict structural parameters within milliseconds and with high accuracy. Hybrid datasets (simulated + synthetic) have achieved Mean Absolute Errors (MAE) below 1 nm across more than 20 parameters while maintaining optical consistency [56]. CNNs also generalize beyond training data, producing meaningful predictions in unexplored design regions. Performance is evaluated using metrics such as R^2 scores and validated against full-wave simulations. Transfer learning and fine-tuning further improve adaptability, enabling pretrained models to be repurposed for related tasks with minimal new data [57]. Overall, CNNs significantly advance inverse design by reducing reliance on iterative simulations, improving accuracy, and enabling real-time exploration of large design spaces.

4. Generative Models and Data Augmentation

Generative models are crucial in AI-driven inverse design, addressing the scarcity and high cost of simulation data in photonic and plasmonic research. Conventional approaches using FEM or FDTD solvers limit dataset size and diversity. In contrast, generative models enable synthetic augmentation, expanding datasets while preserving the statistical and physical fidelity of original simulation results, thereby supporting scalable and efficient device optimization.

4.1 Conditional Tabular GAN (CTGAN)

The Conditional Tabular GAN (CTGAN) is a generative model designed for structured tabular data, capable of handling both numerical and categorical variables [58]. Unlike conventional GANs developed for images or audio, CTGAN learns complex multi-modal distributions and supports conditional sampling, enabling generation of synthetic data under specific constraints, such as predefined contrast ratios or transmission ranges. In plasmonics, CTGAN has been applied to produce thousands of structure–performance pairs, greatly accelerating inverse design model training while avoiding additional simulation costs [59].

4.2 Variational Autoencoders (VAEs)

Variational Autoencoders (VAEs) are generative models that encode high-dimensional data into a latent space and decode it back into synthetic samples via probabilistic modeling. Although originally applied to images, VAEs have been adapted for design tasks by representing structural parameters in reduced dimensions. They are effective in generating smooth variations of configurations and are particularly useful for interpolating between designs or exploring sparse regions of the design space [60].

4.3 SMOTE and Classical Oversampling

Alongside generative models, classical oversampling techniques such as SMOTE are applied to balance underrepresented regions in datasets, particularly in classification or bin-based regression tasks [61]. Although less effective than GANs or VAEs in modeling nonlinear dependencies, SMOTE remains valuable when computational resources are limited or dataset dimensionality is low. Combining simulated and synthetic data has been shown to reduce Mean Absolute Error (MAE) by over 30% compared to using simulations alone [62]. Synthetic augmentation also captures rare but physically meaningful configurations, improving robustness and coverage of the design space. Thus, whether through SMOTE or advanced generative models, data augmentation is a core enabler of scalable and accurate AI-driven photonic device design.

5. Hybrid Physics-Informed Models

Although neural networks and tree-based models provide strong predictive power in plasmonic inverse design, they often demand large datasets and lack physical interpretability. To address this, Hybrid Physics-Informed Models integrate machine learning with physical principles. A key example is Physics-Informed Neural Networks (PINNs), which embed PDEs, boundary conditions, and conservation laws into the loss function [63]. In plasmonics, PINNs incorporate Maxwell's equations to ensure physically consistent predictions, reducing dataset dependence and improving generalization to unseen designs [64]. Another strategy is hybrid surrogate modeling, where neural networks are combined with analytical methods such as modal analysis or coupled-mode theory. Here, ML refines empirical coefficients or fills gaps in incomplete models for example, correcting effective index models or capturing dispersion in plasmonic waveguides [65]. While physics-informed models require higher computational effort, they deliver superior interpretability, reliability, and extrapolation. They are less prone to overfitting and can work with smaller datasets, making them valuable where simulations are costly [66]. Recent studies confirm their promise: [67] embedded Maxwell's equations into a neural framework for photonic gratings, reducing prediction errors, while [68] demonstrated improved efficiency over standard deep learning. Thus, hybrid physics-informed approaches represent a breakthrough toward explainable and fabrication-ready AI in plasmonics.

6. Comparative Analysis

6.1. Performance Metrics

Evaluating inverse design methods for plasmonic nanostructures requires a framework that considers accuracy, speed, interpretability, and scalability. Accuracy remains central: AI models are typically assessed using MAE, RMSE, and R^2 scores. Random Forests and MLPs, for instance, achieve MAE below 1 nm and R^2 above 0.9 on balanced datasets, often surpassing conventional FEM/FDTD sweeps in complex design spaces [69]. Speed is another advantage. While FEM or FDTD may take hours or days for a single configuration, trained AI models predict results in milliseconds, reducing design cycles by up to 100×–1000× [70]. Interpretability varies: simulations are fully transparent but slow, tree-based models allow feature importance analysis, whereas deep networks function as black boxes unless aided by explainable AI tools such as SHAP or LIME. Nonetheless, AI models are more robust to noise and incomplete data, and physics-informed networks ensure physical consistency. Finally, scalability strongly favors AI. Unlike solvers that scale poorly with dimensionality, machine learning accommodates large datasets and multi-objective tasks. Generative models like CTGANs and VAEs further expand training data at negligible cost, enabling the design of complex systems such as optical neural networks and quantum interconnects.

6.2. Design Space Coverage

One of the essential things in the analysis of inverse design methodologies for plasmonic devices is their capacity to effectively traverse and cover the design space, and it is more pronounced in high dimensional problems where numerous geometrical and material parameters govern optical performance. In this subsection, we contrast conventional simulation-based workflows and AI-based models based on their capacities for dealing with highly complex, multi-parameter problems of design.

6.2.1 Traditional Methods: Limited Dimensional Scalability

Conventional methods such as FEM and FDTD explore design spaces via parametric sweeps or evolutionary algorithms, systematically varying input parameters to test configurations. While physically rigorous, these approaches face key limitations:

- Computational demand: Adding parameters greatly increases required simulations.
- Time inefficiency: Sweeps beyond 5–7 parameters become impractical due to the curse of dimensionality [71].

- Local minima: Evolutionary algorithms often converge to suboptimal solutions in large spaces [72].

Consequently, traditional workflows are generally limited to low-dimensional optimization, handling only a few parameters (e.g., waveguide width, resonator gap, refractive index) simultaneously.

6.2.2 AI-Based Methods: High-Dimensional Flexibility

Machine learning and deep learning models are naturally suited for high-dimensional design, learning complex nonlinear mappings once trained on sufficient data.

- Random Forest and SVR achieve reliable inverse predictions for 15–20 structural features with sub-nanometer accuracy [73].
- Deep Neural Networks (DNNs) and MLPs scale further, predicting across 20+ variables, including material and geometric parameters as well as spectral responses [74].
- Generative models (CTGAN, VAE) expand design exploration by sampling new, physically consistent configurations beyond those seen in traditional simulations [75].

These capabilities are essential for designing advanced plasmonic devices such as multiplexers, nonlinear switches, and multi-resonator filters, where manual or brute-force optimization would be prohibitively slow and incomplete.

Table 2. Comparison of Inverse Design Approaches in Nanophotonics and Plasmonics

Method	**Max Design Parameters**	**Sampling Strategy**	**Limitations**
FEM/FDTD Parametric Sweep	~5–7	Grid-based or heuristic	Time-intensive; low coverage of design space
Evolutionary Algorithms	~8–10	Genetic or swarm heuristics	Risk of local minima; convergence time
ML Models (RF, SVR)	~15–20	Data-driven prediction	Requires clean, high-quality training data
DNN/MLP	>20	End-to-end supervised learning	Requires large datasets; interpretability challenges
Generative Models (CTGAN, VAE)	N/A (for sampling)	Synthetic data generation	Validity of generated samples must be verified

To unify the quantitative comparison between conventional and AI-based inverse design methodologies, Table 3 summarizes the key computational and accuracy benchmarks for both categories.

Table 3. Quantitative Benchmark Comparison Between Conventional and AI-Based Inverse Design Methods

Reference	Design Approach	Model / Method	Design Variables	Simulation / Prediction Time	Accuracy (MAE / R^2)	Key Advantages & Limitations
[76]	Conventional	Finite Element Method (FEM)	5–7	3–6 hours per run	N/A	High accuracy for complex geometries; very slow for multi-

						parameter sweeps
[77]	Conventional	Finite-Difference Time-Domain (FDTD)	6–10	2–5 hours per run	N/A	Broadband simulation; large memory demand; slow for 3D models
[78]	Conventional	Beam Propagation Method (BPM)	3–5	Minutes per run	N/A	Fast for paraxial optics; not suitable for plasmonic metals
[79]	AI-Based	Deep Neural Network (DNN)	10–15	< 1 second prediction	MAE = 1.2 nm, $R^2 = 0.94$	High accuracy; may overfit small datasets
80]	AI-Based	Convolutional Neural Network (CNN)	> 20	< 1 second prediction	MAE = 0.97 nm	Captures spatial features; high computational cost in training
[81]	AI-Based	CTGAN (Conditional GAN)	N/A (for data generation)	Dataset generation in minutes	$R^2 = 0.92$	Overcomes data scarcity; requires validation of generated samples

Table 3 provides a common quantitative comparison among conventional electromagnetic solvers (FEM, FDTD, BPM) and AI inverse design models (DNN, CNN, CTGAN). Conventional methods offer high physical accuracy but with hours of computation per configuration, which limits large-scale optimization. In contrast to conventional methods, AI-based models offer sub-nanometer accuracy (MAE < 1 nm) and are able to predict optimal structures within milliseconds following training. Moreover, generative models such as CTGAN effectively address the limitation of data by generating physically plausible synthetic data sets. Hence, marrying AI with physics-based simulations results in a hybrid method that offers acceleration and physical interpretability, and hence scalability is significantly improved for future-generation plasmonic and photonic device engineering.

6.3. Fabrication Readiness and Realism

Although AI has accelerated inverse design and enabled exploration of high-dimensional plasmonic structures, practical fabrication remains challenging. Deep learning and generative models often yield non-intuitive geometries that maximize performance metrics such as contrast ratio, insertion loss, and transmission but overlook fabrication constraints, including feature size, layer thickness, and lithography alignment [82]. In some cases, networks generate discontinuous or overlapping patterns beyond current nanofabrication capabilities. To address this, fabrication-aware strategies are being adopted. Physics-Informed Neural Networks (PINNs) and constraint-regularized loss functions guide networks toward manufacturable designs by enforcing smoothness, symmetry, or spacing [83], while post-processing filters refine patterns before fabrication [84]. Material compatibility also limits viability. AI models may propose optimal but impractical materials due to instability or deposition issues. For instance, silver and indium tin oxide (ITO) offer strong plasmonic performance but suffer from chemical and fabrication challenges [85]. Recent approaches integrate fabrication databases and CMOS-compatible material libraries into training, aligning outputs with practical technology nodes [86]. Experimental validations are emerging. Adibnia et al. (2024) confirmed the feasibility of deep learning–predicted nonlinear plasmonic ring resonators, with close agreement between simulated and fabricated results [87]. However, validations remain limited, underscoring the need for standardized benchmarks to assess fabrication readiness.

7. Challenges and Limitations

Despite progress, AI-based inverse design of plasmonic nanostructures still faces challenges concerning data availability, generalization, interpretability, and physical reliability. A key limitation is the absence of standardized, openly accessible datasets. Most works rely on custom, task-specific data, reducing reproducibility and preventing fair benchmarking across algorithms [88]. Unlike computer vision, which benefits from repositories like ImageNet, nanophotonics lacks equivalent shared resources, though early initiatives are emerging [89]. Generalization is another issue: models trained on narrow datasets often fail on unseen structures. For example, those optimized for ring resonators may perform poorly on gratings or multiplexers [90]. While transfer learning and domain adaptation can improve generality, their adoption in photonics remains limited [91]. Interpretability is also problematic, as many deep models behave like “black boxes.” This undermines trust and scientific insight in critical applications. Explainable AI (XAI) methods, including saliency mapping and sensitivity analysis, have been introduced to correlate predictions with physical intuition [92]. Finally, purely data-driven models may generate non-physical results that violate energy conservation or causality. Hybrid approaches, such as Physics-Informed Neural Networks (PINNs) and constraint-regularized models, help enforce physical validity and enhance reliability, though at the cost of added complexity and computational demand [93].

8. Future Research Directions

AI integration in plasmonic inverse design has shown strong potential for efficiency, scalability, and performance, yet several avenues remain open for advancement. One promising direction is reinforcement learning (RL), which optimizes structures through iterative interaction with simulated environments rather than static datasets. RL enables real-time, feedback-driven refinement, allowing exploration of globally optimal and unconventional architectures. It may also support closed-loop, fabrication-aware systems that adapt designs based on experimental feedback [94]. Another priority is the creation of open-access datasets. The absence of standardized repositories hinders benchmarking and reproducibility. Curated databases with diverse geometries, materials, and optical metrics would facilitate transfer learning, fair model comparison, and broader research participation similar to initiatives like ImageNet or the Materials Project [95]. Addressing the “black-box” nature of AI is also crucial. Explainable AI (XAI) methods such as SHAP, LIME, and saliency mapping can clarify how models relate structural parameters to optical metrics, improving trust, identifying failure modes, and guiding physically interpretable designs [96]. Future systems are expected to evolve into real-time, closed-loop pipelines, integrating AI, simulations, and fabrication feedback. In such frameworks, AI-generated designs could be fabricated (e.g., via lithography or nanoimprinting), measured, and iteratively refined with minimal human intervention. Hardware-in-the-loop approaches would further allow dynamic adjustment of optical properties during fabrication, ensuring alignment with target specifications. Together, these directions RL, open datasets, XAI, and adaptive pipelines will define the next stage of AI-driven photonic device design, pushing the field toward practical, scalable, and fabrication-ready technologies.

9. Conclusion

The integration of artificial intelligence (AI) into the inverse design of plasmonic nanostructures marks a transformative advance in nanophotonics. Traditional simulation-based approaches such as FEM and FDTD, though accurate, are computationally intensive and limited in exploring large parameter spaces. In contrast, AI-driven methods including supervised learning, deep neural networks, and generative models enable rapid prediction of structural parameters from optical targets while efficiently navigating high-dimensional design spaces. Literature shows that AI models, particularly when supported by synthetic data generation through CTGAN or variational autoencoders, achieve high accuracy and generalizability. These approaches reduce design cycles by orders of magnitude and enhance optimization quality, offering robustness across diverse performance metrics. Nonetheless, challenges persist. Data scarcity, limited interpretability, and fabrication constraints underscore the need for physics-informed and explainable AI frameworks. The development of standardized, open-access plasmonic datasets is also essential for benchmarking and advancing future methods. Moving forward, AI should be strategically embedded into nanophotonic workflows, extending beyond prediction to real-time, closed-loop systems integrating simulation, fabrication, and experimental feedback. With continued progress, AI is poised to accelerate and scale the design of plasmonic devices, paving the way for next-generation photonic technologies.

Notation list

Abbreviations	Meaning
k_{spp}	Surface Plasmon Polariton Wavevector
ε_m	Relative Permittivity of Metal
ε_d	Relative Permittivity of Dielectric
$k_\circ$	Free-Space Wavevector ($k_\circ = 2\pi/\lambda$)
L_{SPP}	Propagation Length of SPP
$Im(k_{spp})$	Imaginary Part of k_{spp}, Related to Loss

Declaration of Competing Interest

The authors declare that there are no conflicts of interest regarding the publication of this manuscript.

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