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Inverse Design of Tunable Graphene-Based Terahertz Metasurfaces via Deep Neural Network and SHADE Algorithm

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Abstract

The terahertz (THz) frequency range holds critical importance for next-generation, wireless communications and biomedical sensing applications. However, conventional metamaterial design approaches suffer from computationally intensive simulations and optimization processes that can extend over several months. This work presents an intelligent inverse design framework integrating deep neural network (DNN) surrogate modeling with success-history-based adaptive differential evolution (SHADE) for tunable graphene-based THz metasurfaces. Our DNN surrogate model achieves an exceptional coefficient of determination ($R^2 = 0.9984$) while providing a four-order-of-magnitude acceleration compared with conventional electromagnetic solvers. The SHADE-integrated framework demonstrates 96.7% accuracy in inverse design tasks with an average convergence time of 10.2 s. The optimized configurations exhibit significant tunability through graphene Fermi level modulation, as validated by comprehensive electromagnetic field analysis. This framework represents a significant advancement in automated electromagnetic design and establishes a robust foundation for intelligent photonic systems across diverse frequency regimes.

Keywords: terahertz metasurfaces; inverse design; deep neural networks; graphene; SHADE algorithm; electromagnetic optimization; tunable metamaterials



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1. Introduction

The THz frequency range (0.1–10 THz) has garnered significant attention for its promising applications in next-generation wireless communication systems, high-resolution imaging, and biomedical sensing [1,2]. THz radiation possesses unique properties including a non-ionizing nature, high absorption by conducting materials, and facile transmission through most dielectric media, making it particularly suitable for spectroscopic and diagnostic applications [3]. However, the development of efficient THz systems necessitates active components capable of real-time radiation control with rapid response times and cost-effective implementation.

Recent research highlights the transformative role of metasurfaces across a wide range of applications, including imaging, energy harvesting, material reinforcement, terahertz technologies, and optical communications. For instance, Xiaolong et al. [4] demonstrated three-dimensional terahertz confocal imaging with a chromatic metasurface, showcasing its potential for high-resolution noninvasive detection. Wu et al. [5] proposed an ultra-broadband plasmonic perfect absorber based on MXene all-dielectric triple-vertical-ring nanostructures, enabling efficient full-spectrum solar energy harvesting. Along similar

lines, Liu et al. [6] reported a TiN-only metasurface absorber that achieved high-efficiency solar energy harvesting, highlighting refractory plasmonic materials as cost-effective and thermally robust alternatives to conventional noble metals. In the context of multifunctional materials, Li et al. [7] integrated metasurface technology with three-dimensional four-way weaving structures to develop advanced optical reinforcement materials, simultaneously enhancing mechanical robustness and optical performance. Furthermore, Li et al. [8] demonstrated an ultrathin broadband terahertz metamaterial based on single-layer nested patterned graphene, exhibiting excellent tunability and compact integration capability. Beyond these material and device innovations, Huang et al. [9] comprehensively reviewed how metasurfaces empower optical multiparameter imaging, providing versatile platforms for biomedical and sensing applications, while Rong et al. [10] developed a metasurface-based optical neural network, offering promising solutions for next-generation optical communication systems. Collectively, these works underscore the expanding potential of metasurfaces as enabling platforms that bridge fundamental optical physics with practical applications across diverse domains.

Metamaterials and metasurfaces, characterized by artificially engineered subwavelength structures, offer unprecedented capabilities for electromagnetic wave manipulation and demonstrate considerable promise for addressing THz application challenges [11,12]. Traditional design approaches for THz metamaterials predominantly rely on equivalent circuit theory, electromagnetic wave theory, and parametric sweeping optimization algorithms [13,14]. These conventional methodologies are characterized by stringent specialization requirements, repetitive processes, and substantial computational overhead, often resulting in significant discrepancies between theoretical predictions and experimental performance.

The inverse design problem—determining optimal structural parameters from desired electromagnetic specifications—represents a particularly formidable challenge in metamaterial development. Traditional electromagnetic design methods demand extensive expertise in electromagnetic theory and typically involve complex iterative processes requiring weeks to months for convergence [15,16]. Furthermore, the high-dimensional parameter spaces inherent to metamaterial structures render exhaustive optimization computationally prohibitive using conventional approaches.

Recent advances in artificial intelligence have opened new paradigms for electromagnetic device design, with machine learning techniques showing remarkable potential for accelerating design processes [17,18]. Deep learning algorithms can establish complex mappings between structural parameters and electromagnetic responses, achieving significant speed improvements over traditional full-wave electromagnetic solvers [19,20]. However, most existing approaches focus exclusively on forward prediction without systematic integration with advanced optimization algorithms.

The optimization of graphene-based metasurfaces presents significant computational challenges due to the inherently high-dimensional, multi-modal, and highly non-convex nature of the electromagnetic design space [21,22]. Traditional evolutionary algorithms, commonly employed in metasurface optimization, each exhibit distinct limitations when addressing these complexities. Genetic algorithms (GAs), while offering good global search capabilities, suffer from slow convergence rates and premature convergence issues in high-dimensional spaces, particularly when geometric and material parameters exhibit strong nonlinear coupling [23]. Particle swarm optimization (PSO) demonstrates fast local convergence but is prone to becoming trapped in local optima, especially in the multi-modal electromagnetic landscapes characteristic of metasurface resonance optimization [24]. Standard differential evolution (DE), although robust for continuous optimization, relies

heavily on manual parameter tuning and often exhibits parameter sensitivity that can significantly impact optimization performance across different problem instances [25].

In contrast, the SHADE algorithm addresses these fundamental limitations through sophisticated adaptive mechanisms specifically suited for electromagnetic optimization challenges [26,27]. Unlike conventional evolutionary algorithms that employ fixed control parameters, SHADE incorporates a memory-based parameter adaptation system that dynamically adjusts both the mutation factor (F) and crossover rate (CR) based on the historical success of previous generations. This adaptive capability proves particularly valuable for metasurface optimization, where optimal parameter combinations vary dramatically across different regions of the design space due to the complex interdependencies between geometric dimensions, material properties, and electromagnetic responses.

Traditional metasurface unit cell designs have predominantly relied on simple geometric configurations to achieve electromagnetic functionalities. Various elementary shapes, including circular [28], rectangular [29] and cross-shaped [30], have successfully demonstrated good absorption performance while facilitating straightforward design and fabrication processes. However, these conventional approaches suffer from fundamental limitations in electromagnetic response flexibility due to their constrained morphological degrees of freedom. Therefore, exploring novel metasurface structures with complex topological configurations has emerged as a promising solution to overcome this limitation. In particular, polygonal parametric encoding methods have attracted increasing attention in recent years. Existing studies have demonstrated that polygonal structures not only enable a stronger multiband independent tuning capability [31], but also contribute to a wider impedance matching range owing to their complex boundary conditions [32].

Tunable metamaterials present additional design complexities, particularly when incorporating active materials such as graphene. Graphene's exceptional electronic properties and voltage-controllable conductivity in the THz range make it an ideal candidate for dynamic electromagnetic control [33,34]. The surface conductivity of graphene can be modulated through electrostatic gating, enabling real-time frequency tuning without mechanical reconfiguration. However, existing inverse design methodologies predominantly focus on passive metamaterial structures with fixed electromagnetic properties, rarely considering the systematic integration of actively tunable materials like graphene into the optimization framework.

To address these fundamental challenges, this work presents a comprehensive inverse design framework that systematically integrates DNN surrogate modeling with SHADE for tunable graphene-based THz metamaterials. The framework employs a polygonal symmetric parametric encoding to ensure comprehensive design space coverage while maintaining exceptional shape diversity and geometric flexibility.

The core methodology combines a DNN surrogate model optimized for electromagnetic response prediction with the SHADE optimization algorithm. The surrogate model achieves exceptional accuracy while providing a four-order-of-magnitude speed improvement over rigorous electromagnetic solvers, enabling efficient exploration of the eight-dimensional parameter space. The polygonal encoding methodology ensures high sample diversity and significantly expands the achievable shape gamut beyond conventional geometric configurations.

Experimental validation demonstrates a 96.7% accuracy in inverse design tasks with rapid convergence characteristics. The optimized graphene-integrated metasurface configurations exhibit systematic frequency tuning capabilities through Fermi level modulation, demonstrating predictable red-shift behavior of primary resonance features and substantial amplitude modulation with modulation depths reaching 70%. This framework establishes

a robust foundation for next-generation intelligent photonic design systems with broad applicability across frequency regimes.

2. Materials and Methods

2.1. Structure Design

2.1.1. Metasurface Architecture Overview

The metasurface studied in this work consists of periodic square unit cells with a side length of $P_x = P_y = 330 \text{ } \mu\text{m}$, forming a regular array structure as shown in Figure 1. Each unit cell comprises a three-layer structure: an amorphous silicon (a-Si) top layer with a thickness of $H_1 = 100 \text{ nm}$, a monolayer graphene sheet of $H_2 = 1 \text{ nm}$ thickness placed beneath the a-Si layer, and a bottom silicon dioxide (SiO_2) substrate with a thickness of $H_3 = 115 \text{ nm}$. The cross-sectional view is presented in Figure 2a.

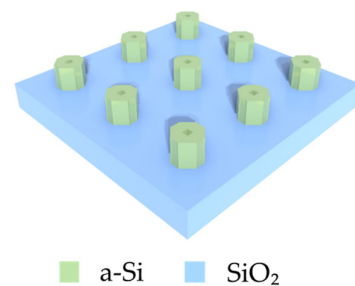


Figure 1. Diagram of the periodic metasurface geometry.

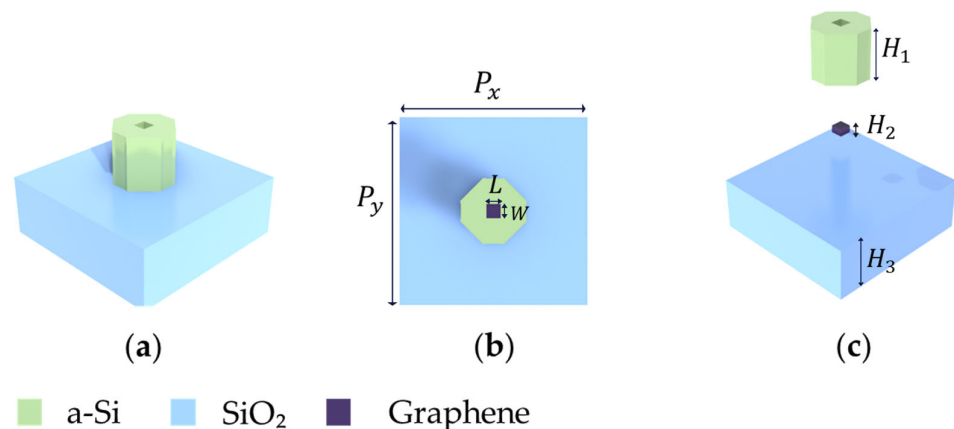


Figure 2. Detailed geometry of a single metasurface unit cell: (a) Side view showing the three-layer structure with a-Si top layer, graphene interlayer, and silicon dioxide substrate; (b) top view illustrating the polygonal symmetric design of the etched a-Si layer with a centrally positioned rectangular graphene patch; (c) layered structure view displaying the spatial arrangement and thickness distribution of all constituent materials.

The geometric design of the metasurface follows an eight-fold rotationally symmetric pattern, in which the a-Si layer is etched into a polygonal configuration to achieve high symmetry and a polarization-insensitive electromagnetic response as shown in Figure 2b. The embedded graphene patch is rectangular measuring $L \times W = 25 \text{ } \mu\text{m} \times 25 \text{ } \mu\text{m}$, centrally positioned within the etched a-Si structure to modulate its electromagnetic response through tunable surface conductivity. Figure 2c illustrates the complete layered architecture, displaying the spatial arrangement and relative positioning of each functional layer.

The proposed architecture leverages the complementary properties of each constituent layer: the a-Si layer provides strong electromagnetic field confinement and resonance enhancement, the graphene layer enables dynamic tunability through electrical gating,

and the SiO₂ substrate ensures structural stability and optimal impedance matching. The multilayer configuration is specifically optimized for the terahertz frequency range (0.4–0.8 THz), wherein graphene exhibits exceptional tunability characteristics.

2.1.2. Parametric Encoding Methodology

The polygonal encoding methodology is specifically developed to ensure comprehensive design space coverage while maintaining exceptional shape diversity as shown in Figure 3. This parametric approach ensures that the generated metasurface configurations span a broad spectrum of geometric possibilities, from highly symmetric structures to complex asymmetric geometries, thereby maximizing the exploration potential for electromagnetic optimization.

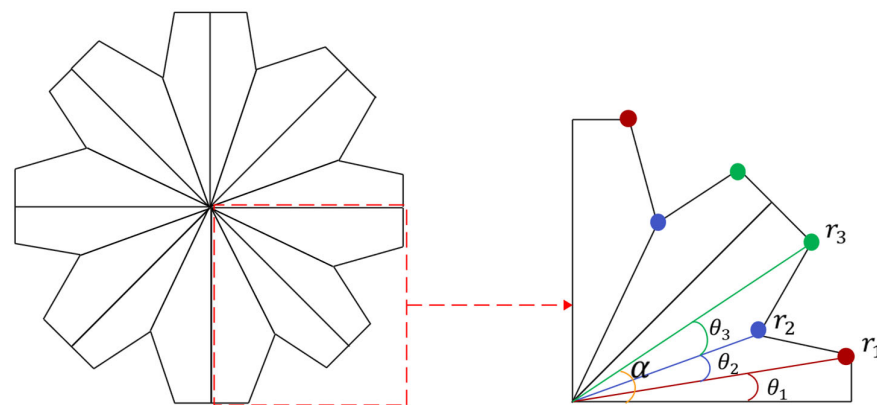


Figure 3. Polygonal symmetric parametric encoding scheme for metasurface unit cell representation.

The geometric parameters are bound within physically meaningful ranges: radial parameters r_1 , r_2 , and r_3 span 25–155 μm ; angular parameters $\theta_i = \frac{\Phi_i}{\sum_{i=1}^3 \Phi_i} \alpha$, where the weights Φ_i are chosen from 10 to 100, while the unit cell periodicity parameter α varies within the interval $[0, \pi/4]$. These parameter bounds are carefully selected to encompass fabricable geometries while maintaining electromagnetic functionality within the operational frequency range.

This polygonal encoding methodology exhibits exceptional compatibility with deep learning architectures employed for electromagnetic response prediction. The fixed-dimensional parameter vector format enables direct input to neural network models without requiring complex preprocessing or dimensional adaptation procedures. The bounded parameter ranges facilitate effective input normalization strategies that enhance training stability and convergence characteristics.

2.2. Graphene Modeling

The electromagnetic response of graphene in the THz frequency range is fundamentally governed by its unique electronic properties arising from the linear energy-momentum dispersion relation of massless Dirac fermions [33]. The surface conductivity of graphene is most accurately described by the Kubo formulation [35], which provides a rigorous quantum mechanical framework for calculating the frequency-dependent optical conductivity based on the electronic band structure and quantum statistical mechanics.

The Kubo formula represents the gold standard for modeling graphene's electromagnetic response, particularly in nanophotonic applications where the accurate prediction of light-matter interactions is crucial for device performance optimization. This theoretical approach has been extensively validated through experimental measurements across multiple research groups and is now widely adopted in commercial electromagnetic simulation software packages [36]. The formulation's accuracy stems from its rigorous treatment of

both classical and quantum mechanical contributions to the optical response, encompassing intraband and interband electronic transitions within a unified theoretical framework.

The total surface conductivity of graphene comprises contributions from both intraband and interband electronic transitions [37,38]:

$$\sigma_g(\omega, T, \tau, E_f) = \sigma_{intra}(\omega, T, \tau, E_f) + \sigma_{inter}(\omega, T, \tau, E_f) \quad (1)$$

where ω is the angular frequency, T is the ambient temperature, E_f is the Fermi energy level, and $\tau = (\mu_v E_f)/(eV_f^2)$ is the relaxation time which can be tuned by the Fermi energy. Graphene exhibits a Fermi velocity V_f of 10^6 m/s, and μ_v is the carrier mobility, which decreases with the carrier density increasing. Experimental observations reveal mobility values spanning $2000\text{--}40,000$ $\text{cm}^2 \text{V}^{-1} \text{s}^{-1}$; for computational simplicity, we adopt an intermediate value of 5000 $\text{cm}^2 \text{V}^{-1} \text{s}^{-1}$ in our analysis [39,40].

The intraband conductivity, which dominates in the terahertz frequency regime, describes the free-carrier response resulting from electron transitions within the same energy band:

$$\sigma_{intra}(\omega, T, \tau, E_f) = j \frac{e^2 k_B T}{\pi \hbar^2 (\omega - j\tau^{-1})} \left[\frac{E_f}{k_B T} + 2 \ln \left(e^{-\frac{E_f}{k_B T}} + 1 \right) \right] \quad (2)$$

where k_B is the Boltzmann constant and $\hbar$ is the reduced Planck constant.

This expression exhibits a Drude-like behavior at low frequencies, where the conductivity is predominantly determined by the chemical potential and scattering mechanisms. These intraband transitions dominate the optical response below 20 THz, making them the primary mechanism for terahertz applications.

The interband conductivity accounts for vertical electronic transitions between the valence and conduction bands:

$$\sigma_{inter}(\omega, T, \tau, E_f) = j \frac{e^2}{4\pi \hbar} \ln \left(\frac{2|E_f| - (\omega + j\tau^{-1})\hbar}{2|E_f| + (\omega + j\tau^{-1})\hbar} \right) \quad (3)$$

For electromagnetic simulations, the surface conductivity must be converted to an effective dielectric constant. The relative permittivity of graphene is given by [41]:

$$\varepsilon_g = 1 + \frac{j\sigma_g}{\varepsilon_0 \omega t_g} \quad (4)$$

where ε_0 is the vacuum permittivity, and t_g is the effective thickness of the graphene layer.

The effective thickness parameter t_g represents a critical modeling consideration, as graphene is inherently a two-dimensional material with atomic-scale thickness (approximately 0.335 nm). However, for computational convenience in three-dimensional electromagnetic solvers, an effective thickness must be specified. Various approaches have been employed in the literature, including setting t_g equal to the van der Waals thickness (0.335 nm), the graphene interlayer spacing in graphite, or optimizing the thickness to match experimental optical constants. To determine the optimal effective thickness for our terahertz metasurface application, we conducted a comprehensive parametric analysis across four representative thickness values: 0.335 nm (van der Waals thickness), 1 nm, 2 nm, and 3 nm, as illustrated in Figure 4. The comparative study reveals a fundamental trade-off between frequency tunability and transmission amplitude variation.

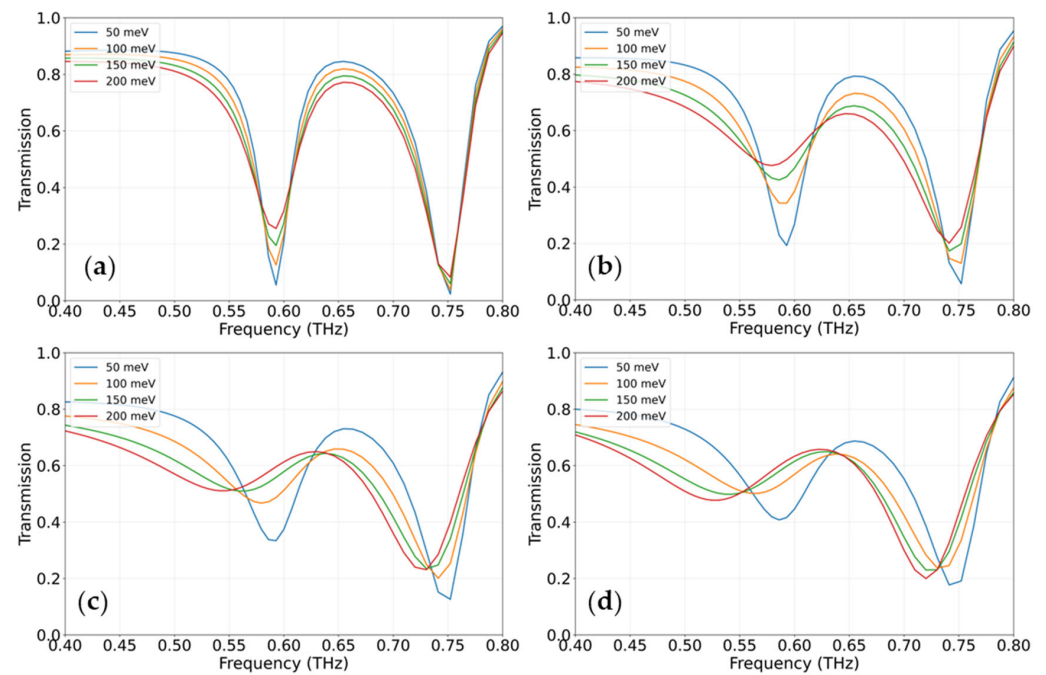


Figure 4. Parametric analysis of graphene effective thickness on transmission spectra tunability across four Fermi energy levels: (a) $t_g = 0.335$ nm; (b) $t_g = 1$ nm; (c) $t_g = 2$ nm; and (d) $t_g = 3$ nm.

As shown in Figure 4, increasing the graphene thickness from 0.335 nm to 3 nm leads to an enhanced frequency modulation capability, with more pronounced spectral shifts observed across different Fermi energy levels. However, this enhancement comes at the cost of reduced transmission amplitude variations, where the transmission variation range progressively narrows from approximately 0.1–0.9 (0.335 nm) to 0.2–0.8 (3 nm).

Specifically, the 1 nm configuration demonstrates an optimal balance between these competing factors, maintaining a substantial frequency modulation capability while preserving a wide transmission variation range (0.1–0.9). This characteristic is particularly advantageous for practical applications requiring both spectral tunability and high signal modulation depth. The 2 nm and 3 nm configurations, while offering superior frequency tunability, exhibit significantly constrained transmission ranges that may limit their effectiveness in amplitude-sensitive applications.

In this work, we adopt an effective thickness of $t_g = 1$ nm [42,43], which represents an optimal compromise between computational stability, physical accuracy, and device performance. This choice not only follows established practices in terahertz metasurface modeling but also maximizes both the frequency tunability and transmission modulation depth of the metasurface, ensuring superior overall electromagnetic performance.

The graphene conductivity model incorporates several critical dependencies that govern the electromagnetic response under various operating conditions. In this work, electrostatic gating serves as the primary mechanism for dynamic Fermi energy modulation, enabling real-time tunability of the metasurface electromagnetic characteristics. The Fermi energy is modulated through electrostatic gating configurations, where applied gate voltages induce controlled charge carrier density variations in the graphene layer. This electrostatic approach enables dynamic tunability with response times primarily limited by the RC (Resistance–Capacitance) time constant of the gating structure [44]. In a typical graphene conductivity model, gate voltages in the range of approximately -100 V to $+100$ V can be readily applied without dielectric breakdown. Owing to the gate capacitance, such a voltage span corresponds to a carrier density modulation of up to approximately $2\text{--}4 \times 10^{12} \text{ cm}^{-2}$. This translates into a Fermi energy shift of about -0.5 eV to $+0.5$ eV [45–47].

The thermal broadening term in Equation (2) introduces temperature-dependent modifications to the conductivity spectrum. At ambient conditions (300 K), thermal excitation leads to Fermi edge broadening and additional loss mechanisms arising from enhanced phonon scattering. While previous studies have demonstrated that cryogenic temperatures can significantly improve conductivity and reduce optical losses in graphene-based terahertz devices [48], all simulations in this work are conducted at 300 K to reflect practical operating environments. In most real-world applications of tunable metasurfaces—including wireless communications, biomedical sensing, and on-chip photonic systems—operation under cryogenic conditions is impractical. Consequently, modeling at room temperature ensures that the proposed design methodology and surrogate model maintain high practical relevance and broad applicability for realistic deployment scenarios.

Figure 5 illustrates the permittivity of graphene as a function of Fermi energy across the terahertz frequency range. The results clearly demonstrate that variations in Fermi levels lead to significant modulations of both the real and imaginary components of graphene conductivity. This conductivity modulation directly translates to changes in the graphene dielectric constant according to Equation (4), establishing the fundamental basis for electrical tunability of the metasurface electromagnetic response. The substantial conductivity variations observed across different Fermi energy levels validate the potential for achieving dynamic spectral control through electrostatic gating, which serves as the core mechanism for the tunable device operation presented in this work.

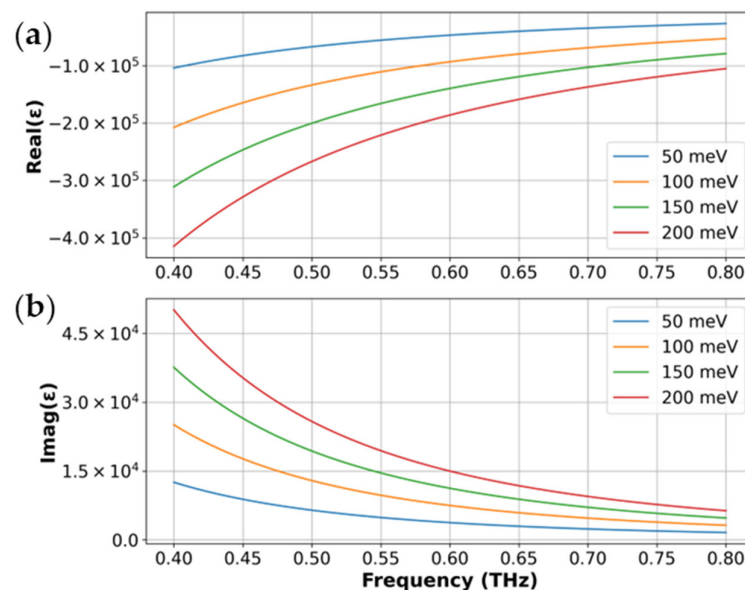


Figure 5. Permittivity of graphene as a function of terahertz frequency for different Fermi energy levels (50 meV, 100 meV, 150 meV, and 200 meV): (a) real part of permittivity; (b) imaginary part of permittivity.

2.3. Surrogate Model Construction

2.3.1. Deep Neural Network Framework for Electromagnetic Response Prediction

Conventional electromagnetic simulation approaches present prohibitive computational burdens for large-scale metasurface design optimization. Full-wave solvers typically require several minutes to hours for a single structural evaluation, making direct optimization strategies impractical when thousands of candidate designs must be evaluated.

To address these limitations, we employ a DNN surrogate modeling approach that establishes empirical mappings between geometric parameters and electromagnetic responses. This data-driven paradigm enables rapid electromagnetic response prediction while maintaining accuracy comparable to rigorous computational electromagnetics meth-

ods. The approach leverages the universal approximation theorem, ensuring that sufficiently deep networks can capture the complex nonlinear relationships between structural parameters and electromagnetic characteristics in metasurface systems.

The DNN framework employs supervised learning to map the 8-dimensional input parameter space $P = [r_1, r_2, r_3, \theta_1, \theta_2, \theta_3, a, E_f]$ to the 64-dimensional electromagnetic response space, comprising 32 transmission coefficients and 32 reflection coefficients corresponding to discrete frequency sampling points across the operational bandwidth. The selection of these eight parameters is based on their collective ability to comprehensively cover the metasurface design space. The seven geometric parameters ($r_1, r_2, r_3, \theta_1, \theta_2, \theta_3, a$) provide sufficient degrees of freedom to generate diverse polygonal configurations that span the full range of achievable electromagnetic responses, while the Fermi energy (E_f) enables dynamic tunability through graphene conductivity modulation. This parameterization strategy ensures that our 100,000 training samples adequately represent the complete performance space of the metasurface, allowing the deep neural network to develop robust generalization capabilities. Unlike traditional theoretical modeling that requires explicit formulation of parameter coupling effects, our data-driven approach allows the neural network to automatically learn these complex interdependencies from the electromagnetic simulation data, eliminating the need for manual analysis of parameter interactions. This approach enables comprehensive design space exploration with substantial computational efficiency improvements compared with direct electromagnetic simulation methods.

High-fidelity electromagnetic simulations constituting the ground truth dataset are performed using the Stanford Stratified Structure Solver (S^4) [49], a state-of-the-art computational electromagnetics framework implementing rigorous coupled wave analysis (RCWA) with scattering matrix formalism. The S^4 solver provides superior convergence characteristics for complex periodic structures through adaptive spatial harmonic truncation, enhanced numerical stability algorithms, and optimized computational kernels. All electromagnetic simulations employ 50 plane wave basis functions in S^4 , providing an effective spatial resolution of 6.6 μm , which corresponds to 60–120 grid points per wavelength in our 0.4–0.8 THz operating range. Periodic boundary conditions are implemented for the 330 $\mu\text{m} \times 330 \mu\text{m}$ square lattice with normal incidence excitation, ensuring that electromagnetic fields satisfy Bloch periodicity at unit cell boundaries. This resolution ensures adequate sampling of the polygonal metasurface geometries while maintaining computational efficiency for the large-scale dataset generation required by the deep learning framework. Material losses are incorporated through the comprehensive Kubo formulation for graphene, which accounts for both intraband and interband electronic transitions ($\sigma_g = \sigma_{intra} + \sigma_{inter}$). The amorphous silicon and SiO_2 substrates are treated as lossless, an approximation supported by experimental measurements demonstrating low loss tangent values for high-quality dielectric materials in the THz frequency range [50,51].

A total of 100,000 training samples is generated through stratified random sampling across the eight-dimensional parameter space consisting of seven geometric parameters ($r_1, r_2, r_3, \theta_1, \theta_2, \theta_3, a$) and one material parameter (E_f). The stratified sampling approach divides each parameter dimension into equal intervals: radial parameters (r_1, r_2, r_3) are sampled uniformly within [25, 155] μm , angular parameters ($\theta_1, \theta_2, \theta_3$) are calculated as $\theta_i = \frac{\Phi_i}{\sum_{i=1}^3 \Phi_i} \alpha$, where the weights Φ_i are chosen from 10 to 100, while the unit cell periodicity parameter a varies within the interval $[0, \pi/4]$, and the Fermi energy E_f is discretely sampled at four fixed values (50, 100, 150, and 200 meV). This sampling strategy ensures uniform distribution across the geometric parameter space while systematically covering the key graphene conductivity states, minimizing clustering effects that could lead to biased training data. Each sample undergoes rigorous electromagnetic simulation using the S^4 solver to compute transmission and reflection coefficients at 32 frequency

sampling points within the 0.4–0.8 THz operational bandwidth. The dataset is partitioned using stratified sampling, allocating 80,000 samples (80%) for neural network training and 20,000 samples (20%) for independent validation and testing. To clarify the computational resources, the generation of 100,000 training samples was executed on a 32-core AMD EPYC 9654 CPU with 60 GB memory. The total computational time required was approximately 111 h, which represents a significant but feasible computational investment for creating the comprehensive training dataset. This time investment enables the generation of high-quality electromagnetic simulation data covering the full parameter space of the metasurface designs, providing the foundation for robust deep learning model training.

2.3.2. Network Architecture

The surrogate model employs fully connected DNN architecture specifically designed for electromagnetic response prediction in metasurface systems. The network architecture comprises 18 layers: 1 input layer, 16 hidden layers, and 1 output layer, as illustrated in Figure 6. This deep architecture was selected to capture the complex nonlinear mappings between geometric parameters and electromagnetic responses in periodic structures.

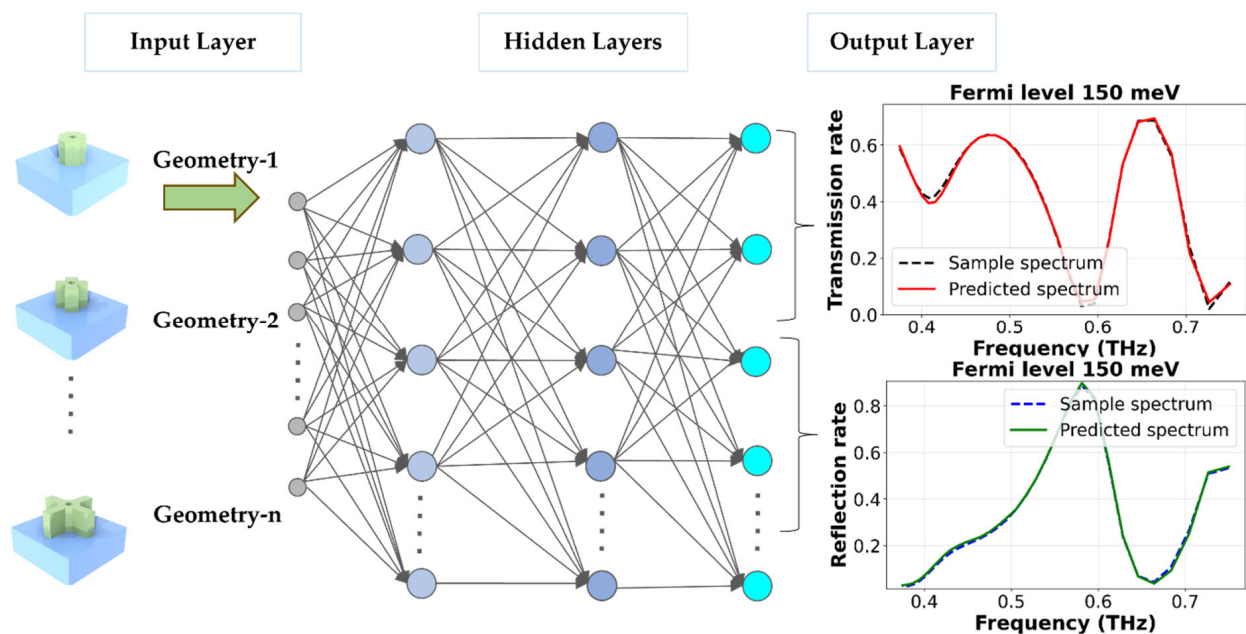


Figure 6. Deep neural network architecture for electromagnetic response prediction.

The input layer accommodates an eight-dimensional parameter vector consisting of seven geometric descriptors ($r_1, r_2, r_3, \theta_1, \theta_2, \theta_3, a$) derived from the polygonal encoding methodology and one material parameter representing the Fermi energy level of graphene. This parameterization effectively addresses the high-dimensional optimization challenge while preserving essential design flexibility.

Each hidden layer contains 512 neurons with rectified linear unit (ReLU) activation functions:

$$f(x) = \max(0, x) \quad (5)$$

The ReLU activation function is well-suited for modeling sharp resonance features commonly observed in electromagnetic metasurface responses. Batch normalization is applied after each hidden layer to stabilize training dynamics, while dropout regularization (dropout probability = 0.2) is applied to the first 12 hidden layers to prevent overfitting.

The output layer generates a 64-dimensional spectral response vector comprising 32 transmission and 32 reflection coefficients across the operational frequency range

(0.4–0.8 THz). Sigmoid activation functions are applied to constrain predicted values within the physically valid range [0, 1]:

$$f(x) = \frac{1}{1 + e^{-x}} \quad (6)$$

The network weight initialization follows the Xavier initialization scheme [52], which scales initial weights according to the number of input and output connections for each layer. This initialization strategy ensures balanced gradient flow during the early training phase and prevents activation saturation that could impede learning convergence. Bias parameters are initialized to small random values to break symmetry while avoiding large initial activations that could destabilize training dynamics.

Advanced optimization techniques, including learning rate scheduling and gradient clipping, are employed to enhance training stability and convergence characteristics. The learning rate schedule implements exponential decay with an initial rate of 0.001, a decay factor of 0.95, and decay steps of 1000 iterations, providing aggressive initial learning followed by fine-tuning in later training phases. Gradient clipping with a maximum norm of 1.0 prevents exploding gradient problems that may occur in deep networks when training on electromagnetic response data with sharp spectral features.

2.4. Optimization Strategy

2.4.1. SHADE Algorithm

The optimization process employs the SHADE [26] algorithm, an advanced variant of differential evolution that addresses the parameter tuning challenges inherent in classical evolutionary algorithms. Unlike conventional differential evolution approaches that require manual parameter configuration, SHADE implements an adaptive parameter control mechanism based on historical success information, thereby eliminating the requirement for empirical parameter tuning and enhancing optimization robustness across diverse problem landscapes.

The SHADE algorithm operates through a sophisticated memory-based adaptation mechanism that maintains the historical records of successful parameter combinations and dynamically adjusts control parameters based on past performances. The algorithm maintains two critical memory banks: M_{CR} for crossover rate history and M_F for mutation factor history, each containing H entries where H represents the memory size. These memory banks serve as repositories of successful parameter configurations that guide subsequent parameter generation and adaptation. In this work, the memory size is set to $H = 10$, enabling each memory bank to store the 10 most recent successful parameter values.

The SHADE algorithm initiates with random population generation within the defined parameter bounds, followed by iterative improvement through mutation, crossover, and selection operations. The adaptive parameter generation mechanism represents the core innovation of SHADE, wherein control parameters are dynamically generated based on historical success patterns rather than static configurations.

The crossover rate CR_i for each individual i is generated through normal distribution sampling centered on a randomly selected memory entry:

$$CR_i = \text{randn}_i(M_{CR,r_i}, 0.1) \quad (7)$$

where r_i represents a randomly selected memory index from $[1, H]$, and the distribution parameters ensure appropriate exploration–exploitation balance.

Similarly, the mutation factor F_i follows a Cauchy distribution:

$$F_i = \text{randc}_i(M_F, r_i, 0.1) \quad (8)$$

The memory update mechanism constitutes a crucial component of the SHADE algorithm, where successful parameter combinations are recorded and integrated into future generations. When a trial vector successfully outperforms its parent, the corresponding CR_i and F_i values are stored in temporary success sets S_{CR} and S_F . The memory banks are subsequently updated using weighted arithmetic and the Lehmer mean:

$$M_{CR,k,G+1} = \begin{cases} \text{mean}_{WA}(S_{CR}) & \text{if } S_{CR} \neq \emptyset \\ M_{CR,k,G} & \text{otherwise} \end{cases} \quad (9)$$

$$M_{F,k,G+1} = \begin{cases} \text{mean}_{WL}(S_F) & \text{if } S_F \neq \emptyset \\ M_{F,k,G} & \text{otherwise} \end{cases} \quad (10)$$

An index k ($1 \leq k \leq H$) specifies which position in the memory will be updated. Initially, k is set to 1, and it increases with each new memory entry. When k exceeds H , it wraps around and resets to 1. During generation G , the memory entry at position k is updated. However, according to update Equations (9) and (10), if no individual in generation G produces a trial vector superior to its parent (i.e., when $S_{CR} = S_F = \emptyset$), the memory remains unchanged.

The weighted arithmetic mean for crossover rate adaptation incorporates fitness-based weighting:

$$\text{mean}_{WA}(S_{CR}) = \sum_{k=1}^{|S_{CR}|} w_k \cdot S_{CR,k} \quad (11)$$

where the weight w_k is calculated based on fitness improvement:

$$w_k = \frac{\Delta f_k}{\sum_{k=1}^{|S_{CR}|} \Delta f_k} \quad (12)$$

where $\Delta f_k = |f(u_{k,G}) - f(x_{k,G})|$, $f(u_{k,G})$ is the fitness value of the k -th trial vector, and $f(x_{k,G})$ is the fitness value of the corresponding parent individual.

The Lehmer mean for mutation factor adaptation emphasizes successful parameter values:

$$\text{mean}_{WL}(S_F) = \frac{\sum_{k=1}^{|S_F|} w_k \cdot S_{F,k}^2}{\sum_{k=1}^{|S_F|} w_k \cdot S_{F,k}} \quad (13)$$

Additionally, SHADE incorporates an adaptive archive size mechanism where the archive parameter p_i is dynamically generated for each individual rather than remaining static:

$$p_i = \text{rand}[p_{min}, 0.2] \quad (14)$$

where $p_{min} = 2/N$ ensures that at least two individuals participate in the selection process, and the upper bound of 0.2 follows established optimization guidelines. N represents the population size, which is the total number of individuals in each generation of the evolutionary algorithm.

2.4.2. SHADE Implementation for Metasurface Inverse Design

In the context of electromagnetic metasurface design, the optimization objective is to determine an optimal set of geometric parameters that minimizes the discrepancy between the target and predicted transmission spectra. This inverse design problem presents a high-dimensional, non-convex, and multi-modal search landscape, wherein traditional gradient-based methods often become trapped in local minima and exhibit slow convergence characteristics.

The electromagnetic optimization landscape exhibits several challenging properties that necessitate the use of evolutionary approaches. First, the objective function contains numerous local optima corresponding to different resonance configurations that may partially satisfy the design requirements but fail to achieve global optimality. Second, the parameter space contains discontinuous regions where small geometric variations can result in abrupt spectral shifts, violating the smoothness assumptions underlying gradient-based algorithms. Third, the electromagnetic response exhibits strong sensitivity to geometric variations, resulting in highly nonlinear parameter-to-performance mappings that are analytically intractable.

To address these challenges, the SHADE algorithm is employed in conjunction with the validated deep neural network surrogate model to efficiently explore the solution space. During each generation of the evolutionary process, candidate solutions are evaluated by computing the mean squared error (MSE) between the target and predicted transmission spectra:

$$\text{MSE}(\mathbf{P}) = \frac{1}{N_f} \sum_{i=1}^{N_f} [T_{\text{target}}(f_i) - T_{\text{NN}}(f_i, \mathbf{P})]^2 \quad (15)$$

where $T_{\text{target}}(f_i)$ represents the desired transmission spectrum at frequency f_i , $T_{\text{NN}}(f_i, \mathbf{P})$ denotes the transmission spectrum predicted by the neural network for geometric design parameters $\mathbf{P}$ at frequency f_i , and N_f represents the number of frequency sampling points across the operational bandwidth.

For the metasurface optimization tasks addressed in this work, the SHADE algorithm employs a population size of 210 individuals, balancing global search capability with computational efficiency. The optimization proceeds over 60 generations, which has been empirically validated as sufficient for convergence in the seven-dimensional design space.

The p-best selection mechanism employs a setting of $p = 0.2$, meaning that the top 20% of individuals are eligible for guiding mutation. This configuration encourages both global exploration and local exploitation, thereby avoiding premature convergence while intensifying the search around promising solutions.

Historical memories for adaptive mutation factors (F) and crossover rates (CR) are maintained with a memory size of $H = 10$. These memories are updated using a weighted Lehmer mean derived from successful offspring only, ensuring that adaptation is driven by genuine fitness improvements rather than random perturbations.

2.4.3. Surrogate-Assisted Evolutionary Optimization Framework

The integration of high-fidelity surrogate models with evolutionary optimization algorithms represents a paradigmatic advancement in computational electromagnetics, enabling efficient exploration of complex design landscapes that were previously computationally intractable.

Building upon the SHADE algorithm foundation established in the previous sections, this work presents a comprehensive surrogate-assisted evolutionary optimization framework that strategically decouples the optimization process from computationally expensive electromagnetic simulations. The framework employs the trained deep neural network as a high-fidelity surrogate model, enabling rapid fitness evaluation while maintaining predictive accuracy comparable to rigorous electromagnetic solvers. This approach transforms the electromagnetic optimization problem from a simulation-intensive task into a data-driven optimization paradigm, wherein the surrogate model provides instantaneous performance predictions across the entire design space.

The complete algorithmic workflow of the proposed surrogate-assisted optimization framework is systematically illustrated in Figure 7. The optimization process begins by

defining the target transmission spectrum, which serves as the reference objective for the inverse design task. Subsequently, the algorithm initializes a population of 210 candidate solutions randomly distributed within the predefined parameter bounds. Simultaneously, the historical memory banks for crossover rates M_{CR} and mutation factors M_F are initialized with default values of 0.5, following established SHADE protocol.

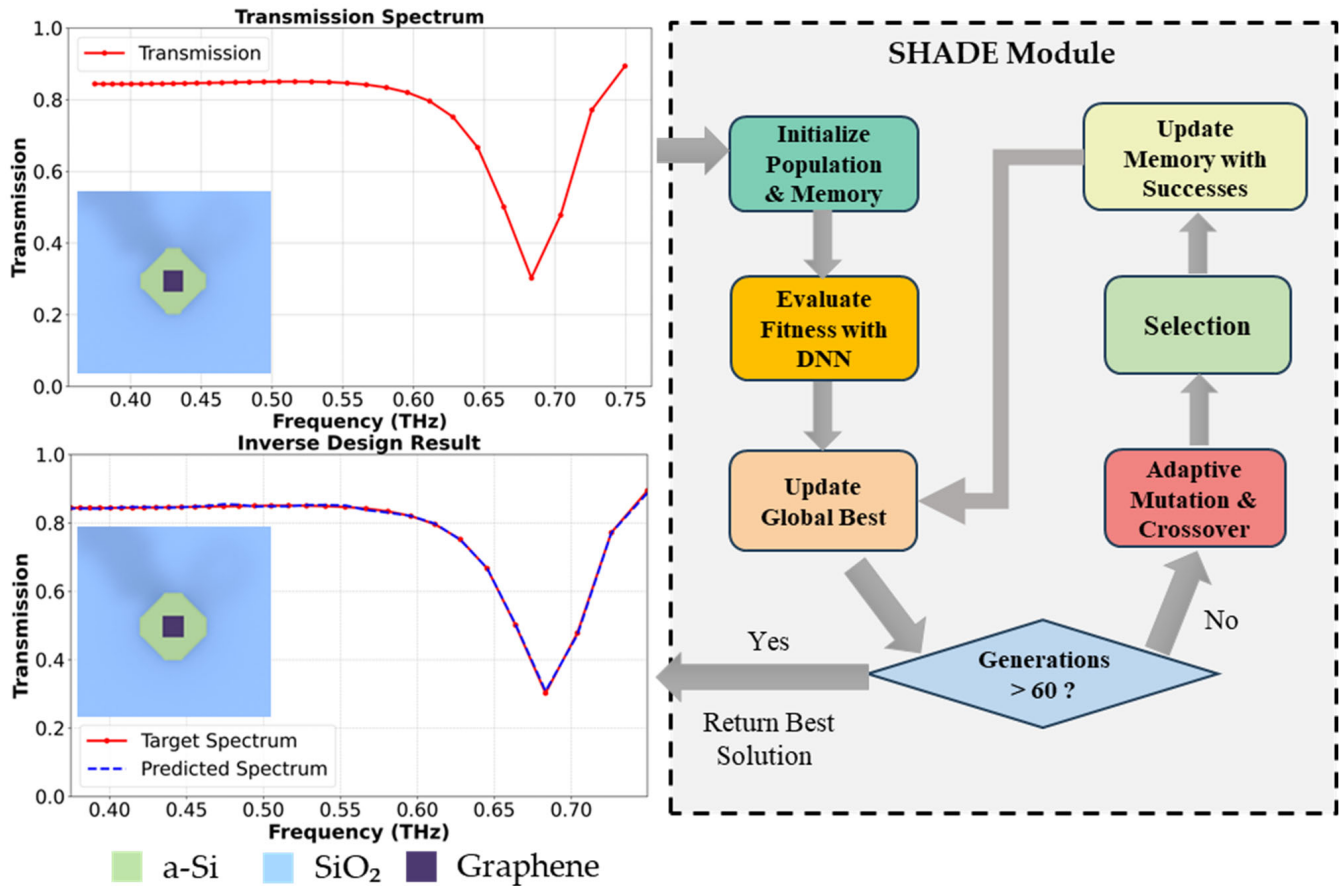


Figure 7. Surrogate-assisted evolutionary optimization framework.

The core optimization loop operates through the following sequential steps: First, each candidate solution undergoes fitness evaluation using the trained DNN surrogate model to predict electromagnetic responses and compute the mean squared error against the target spectrum. The global best solution is continuously tracked and updated whenever superior configurations are identified during the evolutionary process. Second, the algorithm evaluates convergence criteria by checking whether the current generation exceeds the predefined maximum limit of 60 generations or if the fitness improvement falls below a specified threshold.

Upon meeting the termination criteria, the framework returns the optimal design parameters corresponding to the best-performing metasurface configuration. Otherwise, the optimization proceeds through adaptive parameter generation, where mutation factors and crossover rates are dynamically adjusted based on historical success information stored in the memory banks. The SHADE algorithm then executes crossover and selection operations to generate improved offspring solutions, followed by memory bank updates with successful parameter combinations from the current generation.

This optimization framework enables the systematic discovery of metasurface configurations that exhibit desired spectral characteristics while respecting practical fabrication constraints. It demonstrates remarkable flexibility in tailoring key electromagnetic char-

acteristics, such as resonance positions, bandwidths, and peak transmission amplitudes, through the geometric optimization of polygonal resonator configurations.

Moreover, the interpretable nature of the SHADE search process reveals critical design patterns and parameter correlations that govern metasurface response. These insights are valuable for guiding future experimental designs and enhancing the physical understanding of light–matter interactions at the nanoscale.

3. Results and Discussion

3.1. Deep Neural Network Surrogate Model Performance Evaluation

The deep neural network surrogate model demonstrates exceptional predictive performance across the electromagnetic response prediction task, as comprehensively validated through multiple statistical metrics.

The model performance is rigorously quantified through two complementary evaluation metrics formulated in Equations (16) and (17). The MSE, calculated using Equation (16) is as follows:

$$MSE = \frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2 \quad (16)$$

where y_i represents the ground truth electromagnetic response and $\hat{y}_i$ denotes the corresponding network prediction across n sample points.

The coefficient of determination R^2 evolution, calculated using Equation (17), is as follows:

$$R^2 = 1 - \frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{\sum_{i=1}^n (y_i - \bar{y})^2} \quad (17)$$

where $\bar{y}$ represents the mean of the ground truth values.

The comprehensive training analysis reveals optimal convergence characteristics across all performance metrics, confirming the effectiveness of the neural network architecture and training strategy. As shown in Figure 8a, the training and validation loss curves demonstrate consistent convergence behavior, with both metrics decreasing from initial values of approximately 0.37 to final optimized levels below 0.001 within 150 epochs. The absence of significant divergence between training and validation losses confirms a robust generalization capability without overfitting phenomena.

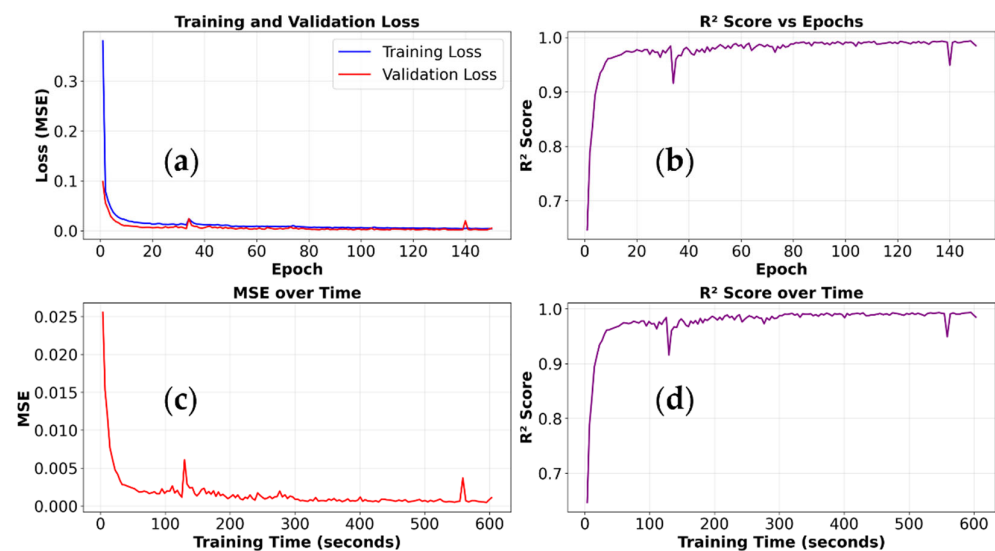


Figure 8. Performance evaluation of the deep neural network surrogate model showing training convergence characteristics: (a) training and validation loss evolution over epoch; (b) R^2 evolution over epochs; (c) MSE reduction over training time; and (d) R^2 evolution over training time.

The R^2 evolution shown in Figure 8b exhibits systematic improvement throughout training, ultimately achieving an exceptional value of $R^2 = 0.9984$. This outstanding performance validates that the deep neural network successfully captures 99.84% of the variance in the electromagnetic response data, with only 0.16% of unexplained variance remaining.

The MSE convergence pattern shown in Figure 8c demonstrates rapid initial improvement, beginning with initial values of approximately 0.025 and converging to a final value of 7.46×10^{-6} . The R^2 evolution over training time presented in Figure 8d further confirms the model's superior predictive capability, demonstrating consistent improvement and stable convergence to exceptional final accuracy.

3.2. Spectral Prediction Accuracy Validation

To validate the surrogate model's predictive capability, representative samples were randomly selected from the test dataset for comprehensive spectral analysis. As illustrated in Figure 9, the DNN predictions for both reflection and transmission coefficients demonstrate excellent agreement with the ground truth values across multiple Fermi energy levels.

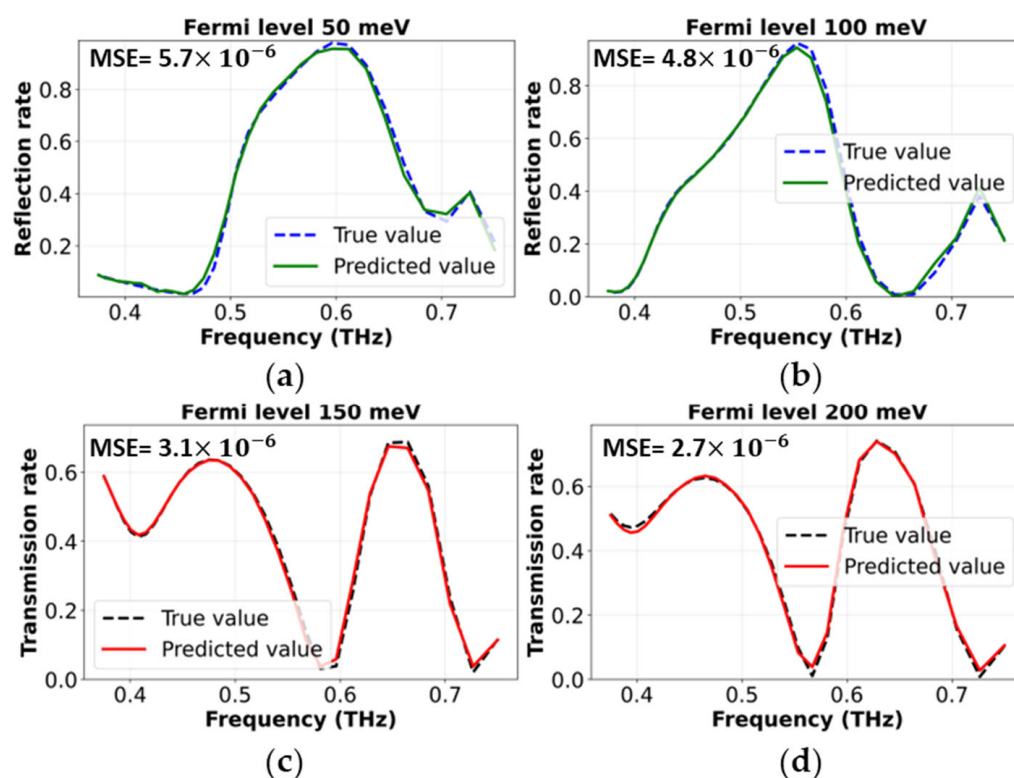


Figure 9. DNN spectral prediction validation showing excellent agreement between predicted and ground truth electromagnetic responses: (a) reflection coefficient comparison at Fermi level 50 meV; (b) reflection coefficient comparison at Fermi level 100 meV; (c) transmission coefficient comparison at Fermi level 150 meV; and (d) transmission coefficient comparison at Fermi level 200 meV.

At Fermi level 50 meV, as shown in Figure 9a, the predicted reflection spectrum (red solid line) exhibits excellent agreement with the S^4 simulation results (black dashed line) across the entire frequency range from 0.40 to 0.80 THz. The model accurately captures the complex reflection behavior, including the characteristic reflection minima around 0.42 THz and 0.68 THz. The quantitative assessment reveals a remarkably low MSE of 5.7×10^{-6} , confirming the exceptional predictive accuracy of the surrogate model at this Fermi energy level.

For Fermi level 100 meV, Figure 9b demonstrates the neural network's remarkable precision in reproducing the complex reflection characteristics. The model accurately predicts the spectral shifts associated with increased graphene conductivity, including the modified reflection minima positions and altered peak amplitudes, validating the model's capability to capture complex electromagnetic interactions under different electrical biasing conditions. The corresponding MSE of 4.8×10^{-6} further substantiates the model's reliability across varying conductivity regimes.

At Fermi level 150 meV, as presented in Figure 9c, the surrogate model successfully predicts the transmission spectral characteristics, accurately reproducing the broadband transmission behavior with characteristic peaks around 0.46 THz and 0.65 THz. The predicted spectrum captures the essential electromagnetic resonance features and bandwidth characteristics associated with graphene conductivity modulation. The achieved MSE of 3.1×10^{-6} demonstrates a consistent predictive performance in the transmission regime.

The 200 meV Fermi level transmission comparison in Figure 9d reveals the model's exceptional capability in modeling complex electromagnetic interactions under elevated chemical potential conditions. The predicted transmission spectrum accurately reproduces the characteristic features, including the pronounced resonance around 0.65 THz and the overall spectral shape profile, validating the model's understanding of the underlying physical mechanisms governing graphene-metasurface interactions. With an MSE of 2.7×10^{-6} , the model maintains high fidelity even under high-conductivity conditions.

To quantitatively demonstrate the computational efficiency of the proposed DNN-based surrogate model, we compared its prediction time with that of the S^4 solver. The results show that the DNN model predicts the electromagnetic response of a single design configuration in approximately 0.6 s, whereas the S^4 solver requires around 15 s for the same task.

3.3. Comprehensive Inverse Design Results

To comprehensively validate the inverse design framework's capability, extensive testing was conducted on 1000 samples to assess the framework's performance across a broad range of target spectra. Four representative samples were systematically selected from this comprehensive test dataset for detailed spectral and structural analysis, as illustrated in Figure 10. The target transmission spectra from these samples were input into the SHADE + DNN optimization framework to determine the corresponding optimal structural configurations, demonstrating the framework's effectiveness in solving complex inverse electromagnetic design problems.

As illustrated in Figure 10, the optimization framework successfully identifies metasurface configurations that produce transmission spectra in excellent agreement with target responses across all test cases. The predicted transmission characteristics accurately reproduce critical spectral features, including resonance peak positions, amplitudes, and bandwidths. The structural comparison reveals remarkable geometric fidelity, with the optimized polygonal resonator configurations closely matching the target designs in terms of radial dimensions, angular parameters, and overall symmetry characteristics. The quantitative evaluation demonstrates exceptional inverse design accuracy, with MSE values of 1.1×10^{-5} , 2.5×10^{-5} , 4.0×10^{-5} , and 1.3×10^{-5} for test samples 1, 2, 3, and 4, respectively. These consistently low MSE values across diverse target spectra validate the robustness and versatility of the SHADE + DNN optimization framework.

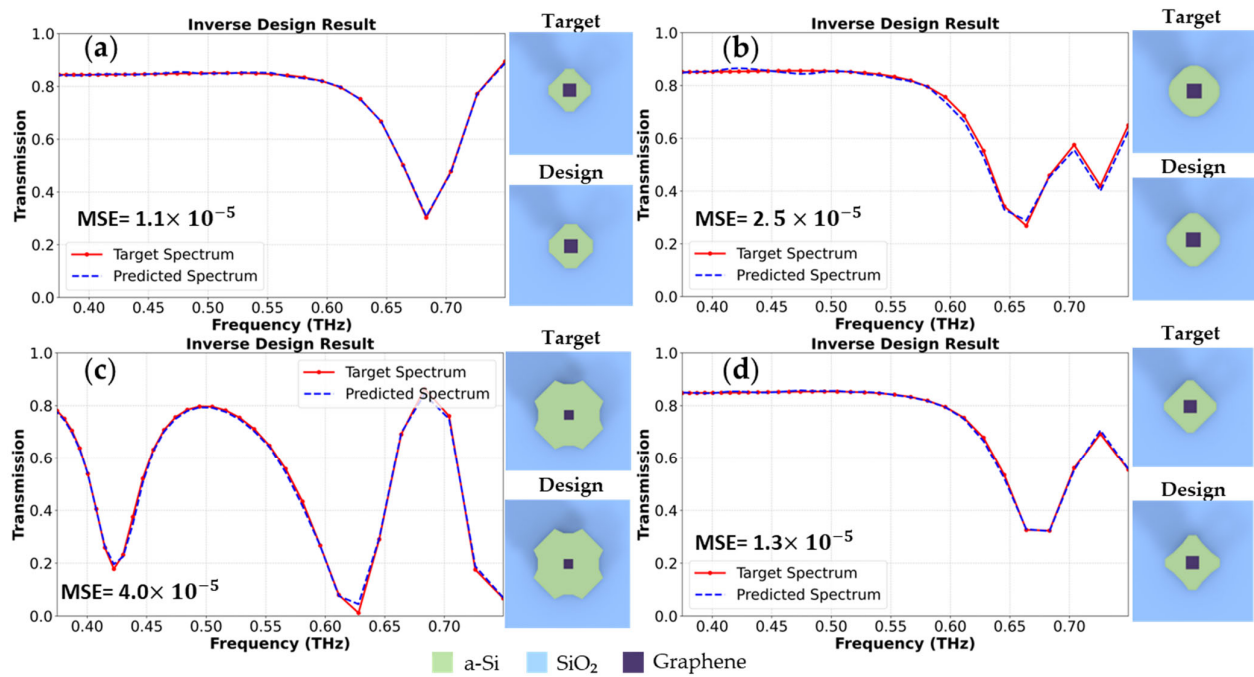


Figure 10. Inverse design framework validation showing target-to-prediction fidelity: (a) Test sample 1; (b) Test sample 2; (c) Test sample 3; and (d) Test sample 4.

Following structural optimization, comprehensive tunability validation was conducted across an expanded Fermi energy range (50–1000 meV) using direct S^4 electromagnetic simulations to address the broader electrostatic tuning capability of the optimized metasurface structures. Four representative structures were selected from the 1000 optimized samples generated by the deep learning framework for detailed analysis. As illustrated in Figure 11, these structures exhibit robust and systematic tunability across the expanded Fermi energy range. The consistent spectral evolution across all four structures validates the generalization capability of the deep learning framework, with each configuration enabling dynamic frequency control through graphene conductivity modulation. All structures demonstrate predictable red-shift behavior of their primary resonance features with increasing Fermi energy, accompanied by substantial amplitude modulation that enables effective transmission control.

To illustrate these tunability characteristics in detail, the transmission spectrum for the optimized structure in Figure 11b serves as a representative example of the exceptional performance achievable through this framework. As the Fermi energy of graphene increased from 50 meV to 1000 meV, the primary resonance around 0.65 THz exhibited systematic red-shift behavior, shifting from approximately 0.67 THz to 0.62 THz. Additionally, a prominent resonance feature around 0.71 THz exhibited substantial amplitude modulation, with transmission values decreasing from 0.6 to 0.18 without significant frequency shifts. This corresponds to a modulation depth ($md = \frac{T_{max} - T_{min}}{T_{max}} \times 100\%$) of 70% at the 0.71 THz frequency point, demonstrating highly efficient electrostatic control over the electromagnetic response. The observed red-shift behavior originates from the interplay between increased graphene conductivity and enhanced ohmic damping, where higher conductivity leads to stronger electromagnetic losses that modify the effective quality factor and resonance conditions of the metasurface unit cells, resulting in systematic frequency downshift.

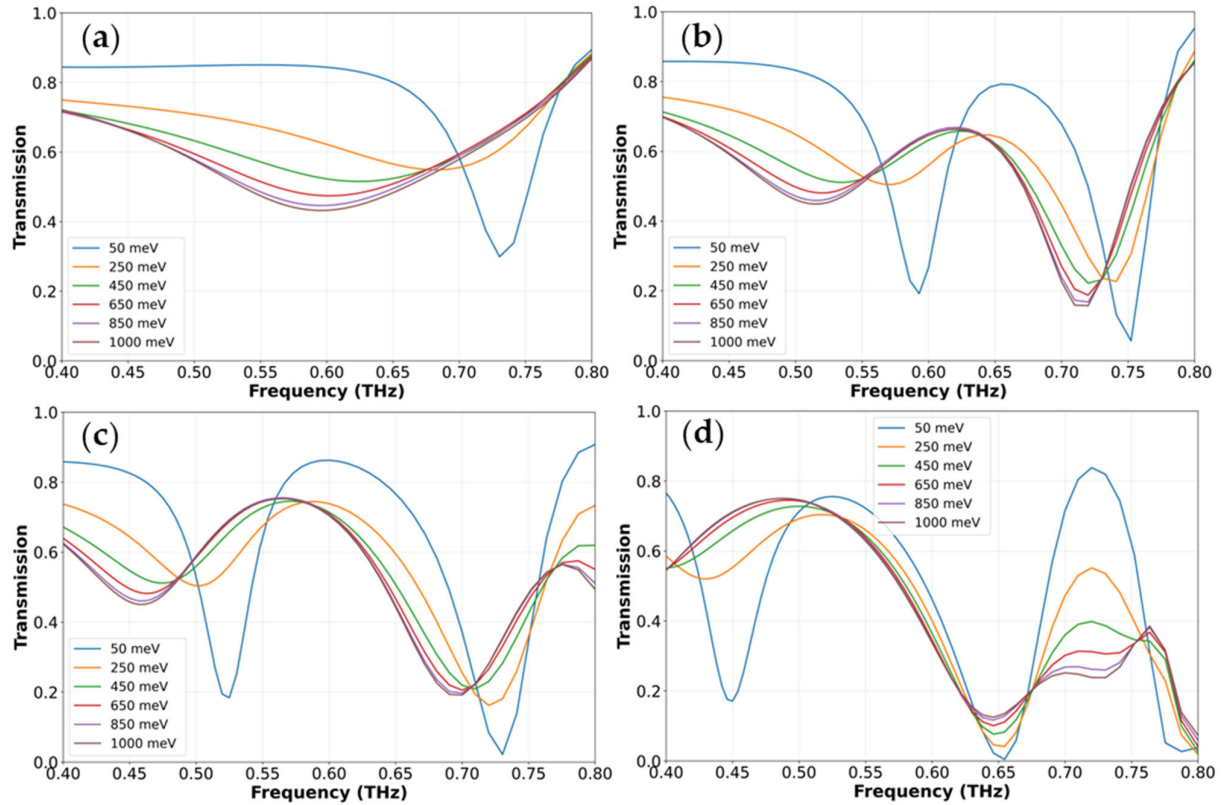


Figure 11. Tunability validation of optimized metasurface configurations across multiple Fermi energy levels: (a) Structure 1; (b) Structure 2; (c) Structure 3; and (d) Structure 4.

The systematic spectral evolution across the extended Fermi level range demonstrates the deep learning framework’s ability to identify metasurface configurations with inherent tunability. The smooth and predictable electromagnetic response progression, characterized by both frequency tuning and amplitude modulation capabilities, confirms that the neural network successfully captured the fundamental structure–performance relationships governing graphene-based metasurface tunability. This comprehensive validation demonstrates the framework’s effectiveness in enabling reliable design optimization for practical electrostatic tuning applications in terahertz frequency manipulation.

3.4. Electromagnetic Field Distribution Analysis and Structural Validation

The electromagnetic field distribution analysis provides critical validation of the optimized metasurface structures obtained through the inverse design framework. Comprehensive electromagnetic simulations were performed using the S^4 solver at an operational frequency of 0.545 THz across different Fermi energy levels. The electric field intensity distributions are presented in normalized units relative to the incident wave electric field magnitude E_0 , enabling a direct comparison of field-enhancement characteristics across the various configurations.

As illustrated in Figure 12, the field distribution analysis reveals systematic electromagnetic enhancement patterns for the optimized structure, with field enhancement originating from surface plasmon polaritons (SPPs) excited at the graphene–dielectric interface [53,54]. The analysis across six Fermi energy levels (50, 250, 450, 650, 850, and 1000 meV) demonstrates a progressive enhancement trend with maximum field intensities increasing from 3.01 to 5.61 times the incident field strength, directly correlating with increasing graphene conductivity and plasmonic response. The observed field-enhancement values (3.01–5.61)

are consistent with the literature reports of field-enhancement factors around $M = 5$ for graphene-based THz metamaterials [55].

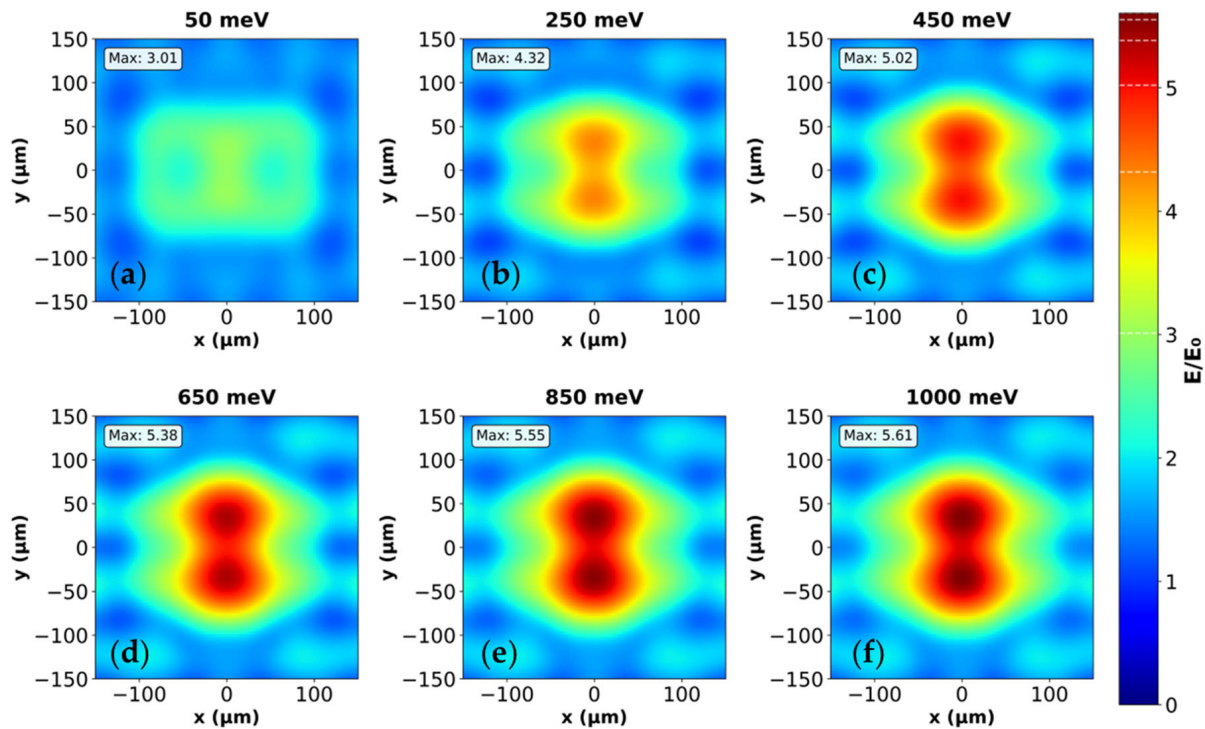


Figure 12. Electromagnetic field distribution analysis of metasurface: (a) field distribution at 50 meV Fermi level; (b) field distribution at 250 meV Fermi level; (c) field distribution at 450 meV Fermi level; (d) field distribution at 650 meV Fermi level; (e) field distribution at 850 meV Fermi level; and (f) field distribution at 1000 meV Fermi level.

3.5. Surrogate-Assisted Optimization Framework Performance Analysis

The integration of the SHADE algorithm with the deep neural network surrogate model demonstrates exceptional computational and predictive performance in tunable terahertz metasurface inverse design applications. To rigorously validate the effectiveness of the proposed SHADE + DNN framework, we conducted comprehensive performance evaluations focusing on the synergistic benefits of combining adaptive evolutionary optimization with high-fidelity electromagnetic response prediction.

For rigorous performance evaluation, we define the accuracy metric used in our comparative analysis. The accuracy represents the proportion of inverse design test cases that successfully achieve the target specifications within acceptable error bounds:

$$Accuracy = \frac{\text{Number of test cases with } MSE < \text{threshold}}{\text{Total test cases}} \times 100\% \quad (18)$$

where the MSE threshold is set to 0.001 based on the acceptable electromagnetic response deviation for practical applications. To validate our framework's performance, we conducted comprehensive testing on 1000 randomly selected samples from the test dataset, achieving an average MSE of 3.4×10^{-5} and an accuracy of 96.7%. This demonstrates that 967 out of 1000 test cases successfully met the design specifications within the predefined error tolerance. The exceptionally low average MSE value, which is significantly below the threshold, confirms the high fidelity of our surrogate model predictions and the effectiveness of the SHADE optimization algorithm in generating accurate metasurface configurations.

The SHADE + DNN framework's performance is evaluated through a systematic comparison with alternative surrogate-assisted optimization approaches commonly employed in electromagnetic design. Table 1 presents the performance metrics obtained from comprehensive benchmarking across multiple inverse design targets.

Table 1. Inverse design framework performance comparison.

Method	Accuracy (%)	Frequency Range	Design Time	Application Domain
REACTIVE [56]	76.51	THz range	200× faster than conventional	General metasurface
DNN (Wide-frequency) [22]	92.0	4–45 GHz	Not mentioned	Wideband metasurface
cDCGAN Global Design [18]	>90	4–12 μm	Not mentioned	Multi-class metasurface
CNN + GA Inverse Design [57]	90.05	0.2–2 THz	10 min	Random metasurface patterns
SHADE + DNN (This work)	96.7	0.4–0.8 THz	10.2 s	Tunable graphene metasurface

As Table 1 verifies, the proposed SHADE + DNN framework not only proves suitable for tunable graphene-based THz metasurface design but also exhibits the advantages of exceptional accuracy (96.7%) and ultra-fast optimization (10.2 s) without requiring extensive parameter tuning. In contrast to conventional inverse design methods, the proposed approach excels in reducing computational overhead, accelerating design convergence, minimizing optimization complexity, and achieving superior tunability performances, while also catering to the specific requirements of electrically tunable THz devices. Therefore, this integrated approach provides an efficient and robust design methodology for tunable THz metasurfaces, which holds promising application prospects in next-generation wireless communications, biomedical sensing, and adaptive electromagnetic control systems.

3.6. Fabrication Feasibility and Process Integration

The proposed graphene-tunable metasurface structure can be realized through established semiconductor fabrication processes combined with proven graphene integration techniques. The polygonal a-Si resonator array can be fabricated using standard CMOS-compatible photolithography and reactive ion etching, with a demonstrated capability for large-area manufacturing on 12-inch wafers [58]. The geometric flexibility required for arbitrary polygonal shapes has been confirmed in recent metasurface fabrication literature [59].

Graphene integration is achieved through established methods that ensure adequate interface bonding quality. The graphene/a-Si interface is stabilized primarily by van der Waals interactions [60], which provide sufficient adhesion for device operation while preserving graphene's electronic properties. The experimental validation of this approach has been demonstrated by Müller et al. [61], who successfully achieved direct a-Si deposition on CVD graphene via PECVD at temperatures as low as 100 °C without compromising graphene characteristics. Additionally, advanced graphene transfer techniques such as the semi-dry transfer method [62] enable clean interface formation with pre-patterned silicon structures, ensuring process compatibility between metasurface fabrication and graphene integration.

While the electromagnetic design principles are thoroughly established in this work, practical implementation requires addressing the electrostatic gating structure design and

optimization, which represents a critical area for future experimental investigation. The sequential processing approach—standard photolithography for polygonal patterning followed by controlled graphene integration—provides a clear pathway for experimental realization of the proposed tunable metasurface concept.

4. Conclusions

This work presents a comprehensive AI-enabled inverse design framework for tunable graphene-based terahertz metasurfaces that successfully addresses the critical challenges of computational efficiency, design space exploration, and tunability range optimization. The developed methodology integrates deep neural network surrogate modeling with the SHADE algorithm, achieving unprecedented performances in both prediction accuracy and design optimization efficiency. The deep neural network surrogate model demonstrates exceptional predictive capabilities with an excellent coefficient of determination (0.9984) and enables electromagnetic response prediction with four-order-of-magnitude speed-up improvements compared with conventional full-wave solvers. The SHADE-based optimization framework achieves a remarkable accuracy of 96.7% in inverse design tasks with an average convergence time of 10.2 s, significantly outperforming existing approaches. The optimized graphene-integrated metasurface configurations demonstrate systematic frequency tuning and amplitude modulation capabilities through electrostatic Fermi level modulations, with representative structures showing predictable red-shift behavior and modulation depths reaching 70%. Furthermore, the framework exhibits excellent generalizability to other tunable metasurface applications and provides a robust foundation for future advances in computational photonics and intelligent electromagnetic design. Future work should focus on uncertainty-aware optimization, multi-objective design strategies, experimental validation, and integration with automated fabrication workflows to fully realize the potential of AI-enabled photonic design.

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