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REVIEW

Reviews of algorithm-driven terahertz metamaterials: From intelligent design to multidisciplinary applications

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Terahertz metamaterials, composed of subwavelength artificial structures, exhibit strongly nonlinear and tightly coupled electromagnetic responses governed by geometry, material properties, and resonance modes. Driven by growing demands in high-sensitivity sensing, terahertz communication, and functional imaging, the design space of these devices has rapidly expanded, rendering conventional empirical and parameter-sweeping approaches inefficient for global optimization. Algorithm-driven strategies, particularly those leveraging machine learning and deep learning, have emerged as powerful surrogates for electromagnetic simulation, enabling automated multi-objective optimization and rapid inverse design. Beyond predictive capabilities, these algorithms uncover latent physical mechanisms and support adaptive, closed-loop experimental implementations. Within a unified framework, this review systematically categorizes and summarizes advances in algorithm-driven design of terahertz metamaterials, including traditional optimization methods, machine learning, deep learning, and reinforcement learning, highlighting their roles in multi-layer structural design, multimodal coupling control, and dynamic multi-target detection. Finally, we conduct a detailed analysis of current challenges, including data quality, model generalization, and physical interpretability, and clearly identify future research directions. These directions are expected to lead to practical applications in high-sensitivity chemical and biological detection, terahertz wireless communication, and wave-based functional imaging.

Keywords: terahertz metamaterials, AI algorithms, intelligent design, applications

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1. Introduction

Metamaterials are a class of electromagnetically functional materials composed of subwavelength artificial structures arranged in a periodic pattern. By leveraging structural design rather than the intrinsic properties of the material, metamaterials can achieve electromagnetic responses that are difficult to obtain with natural materials.[1] Early research focused primarily on unconventional parameters such as negative permittivity and negative permeability, which were validated both theoretically and experimentally.[2–5] With the advancement of micro- and nanofabrication technologies, the scope of metamaterial research has continuously expanded, gradually encompassing multiple fields including acoustics,[6,7] optics,[8,9] and thermodynamics,[10,11] and demonstrating significant application value in areas such as imaging, communications, and sensing. Terahertz (THz) waves, situated between microwave and infrared frequencies, are characterized by their non-ionizing nature, high penetration, and sensitivity to molecular vibrations.[12] These properties confer significant advantages to terahertz technology in fields such as security screening,[13,14] biomedicine,[15,16] non-destructive testing,[17–19] and next-generation wireless communications.[20,21] However, in practical applications, natural materials have limited ability to modulate terahertz waves, and traditional devices typically rely on bulky optical components, making it difficult to meet the demands of system integration and device miniaturization. Therefore, how to achieve efficient modulation of THz waves at the subwavelength scale has become an urgent issue in this field.

THz metamaterials based on artificial microstructures offer an effective solution to this problem. By rationally designing the geometry and arrangement of metamaterial units, strong localized electromagnetic resonance can be generated in the THz band, thereby significantly enhancing the interaction between light and matter. This characteristic gives THz metamaterials unique advantages in high-sensitivity sensing,

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functional imaging, and novel communication devices. At the same time, the integration of metamaterial structures with novel functional materials — such as two-dimensional materials and phase-change materials — further expands their controllable range and application scenarios. However, the electromagnetic response of THz metamaterials is typically determined by a combination of multiple structural and material parameters. There are significant nonlinear relationships among these parameters, and different resonance modes often couple with one another. As device functional requirements increase, the number of design parameters continues to grow, resulting in a high-dimensional design space. Under these conditions, empirical parameter-scanning methods require extensive full-wave simulation calculations, leading to low design efficiency and making it difficult to guarantee globally optimal results. Consequently, the structural design process itself has gradually become a significant factor limiting further improvements in device performance.

Artificial intelligence, as a computing solution that mimics human cognition, is developing rapidly.[22] To improve design efficiency, many studies have begun to incorporate algorithm-assisted design methods, as shown in Fig. 1. Early work primarily employed optimization strategies such as genetic algorithms (GA) and particle swarm optimization (PSO) to achieve specific performance objectives by searching the parameter space.[23–25] While these methods have alleviated the issue of manual parameter tuning to some extent, they still face challenges such as high computational costs and limited scalability when dealing with high-dimensional parameter spaces and multi-objective constraints. At the same time, with improvements in computational power and data acquisition capabilities, machine learning and deep learning methods have gradually been introduced into THz metamaterial design. For example, some studies have combined machine learning methods with flexible manufacturing processes to accelerate the design and fabrication of THz metamaterial absorbers. This work establishes a mapping relationship between structural parameters and absorption performance, using machine learning models to rapidly predict the electromagnetic response of different structures. By integrating droplet printing technology for device fabrication, it reduces the time required for iterative simulations and experiments, thereby improving the design efficiency of flexible THz metamaterial absorbers.[26] Concurrently, other research has introduced deep learning methods into the design of high-dimensional THz devices, proposing a broadband THz photodetector design method based on deep neural networks (DNNs). This method utilizes deep learning models to learn the relationships between complex structural parameters and multi-band response, enabling rapid design and optimization of ultra-wideband and high-dimensional response characteristics, thereby demonstrating the advantages of deep learning in handling high-dimensional parameters and complex optimization problems.[27]

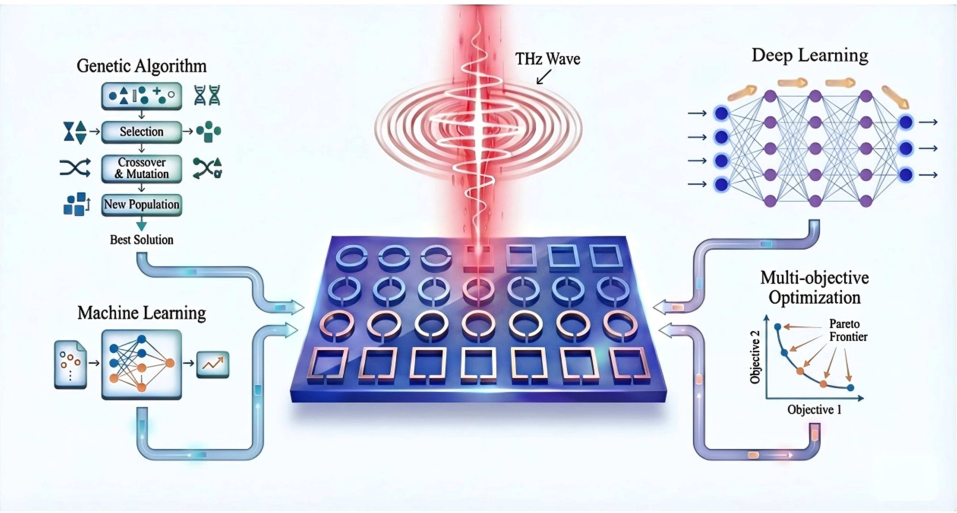


Fig. 1. Algorithm-driven design workflow for THz metamaterials

Data-driven machine learning and deep learning methods can directly learn the mapping relationship between structural parameters and electromagnetic responses, thereby enabling rapid performance prediction and inverse design. These methods reduce reliance on repetitive full-wave simulations and provide new guidance for the automatic generation of complex structures. Against this backdrop, algorithm-driven THz metamaterial design has gradually shifted from traditional optimization toward data modeling and intelligent design, emerging as a major trend in current research.[28] In recent years, as the structural complexity of devices has continued to increase and performance requirements have risen, traditional methods relying on empirical design and parameter scanning have gradually revealed limitations in terms of design efficiency and applicability. Consequently, the introduction of algorithm-assisted design strategies has emerged as a viable and widely

recognized solution, helping to enhance design efficiency and expand the structural design space. Based on the aforementioned developments, this paper focuses on algorithm-driven THz metamaterial design, systematically reviews relevant research, and summarizes the application progress of various algorithms in structural optimization, performance prediction, and inverse design. Additionally, through the synthesis and analysis of typical structural forms, material systems, and application scenarios, the paper further explores the fundamental mechanisms and applicability characteristics of various methods, with the aim of providing valuable references for future research.

2. The physical complexity of terahertz metamaterials

The structural design of THz metamaterials essentially addresses a highly nonlinear, high-dimensional, and strongly coupled physical problem. In the THz band, electromagnetic responses are simultaneously constrained by subwavelength structural resonance, intrinsic material dispersion, and loss mechanisms, such that even a slight change in a single design parameter can cause a significant shift in the overall spectral characteristics. At the material level, the THz band lies at the interface between electronics and photonics. Traditional metallic materials exhibit significant ohmic losses, while conventional dielectric materials have weak electromagnetic responses, making it difficult to achieve high quality factors or strong field localization effects. To overcome this limitation, two-dimensional materials, phase-change materials, and topological materials have been widely incorporated into THz metamaterial systems.[29] However, while the tunability of material properties has expanded functional boundaries, it has simultaneously amplified design freedom, thereby significantly increasing the dimensionality and complexity of the parameter space. At the structural level, to achieve fine-tuned control of THz waves, metamaterial unit dimensions typically need to reach the micrometer or even nanometer scale, where near-field coupling, mode hybridization, and higher-order resonance effects among multiple structural units are prevalent. Consequently, a strong nonlinear and many-to-one mapping relationship emerges between design parameters and electromagnetic response, rendering traditional design strategies based on empirical rules or single-parameter scans ineffective. In terms of performance, bandwidth, quality factor, absorption efficiency, and polarization and incidence angle stability often influence one another. It is difficult to simultaneously satisfy all requirements through manual selection or local adjustments based solely on empirical experience. In contrast, data- and algorithm-driven global optimization is better suited to address these high-dimensional, multi-objective problems. Traditional metals exhibit significant ohmic losses in the THz band, while dielectric materials may struggle to achieve the desired electromagnetic response. Consequently, the exploration of novel materials to reduce losses has become a critical priority.

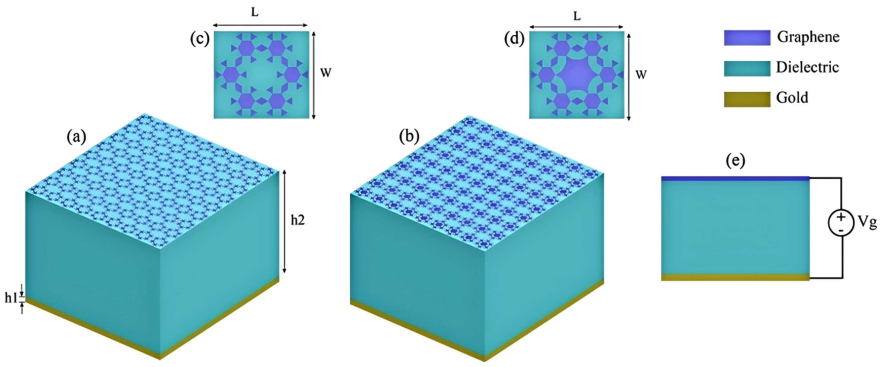


Fig. 2. (a), (b) Perspective views of Penrose absorber models 1 and 2. (c), (d) Top views of Penrose models 1 and 2 within a unit cell. (e) Side view of the proposed model when a bias voltage V_g is applied between the patterned graphene and the bottom gold layer.[31]

As a two-dimensional Dirac material, graphene exhibits significant application potential in THz metamaterials due to its unique electronic properties. For example, Lee *et al.*[30] proposed a highly sensitive biosensing technique based on the combination of graphene and THz nanogap metamaterials for detecting extremely low concentrations of single-stranded DNA (ssDNA). The transmission efficiency of the graphene-nanogap metamaterial designed using this approach can reach up to 52%. This has advanced the application of THz technology in biomedical detection and provided a new perspective for studying the optoelectronic behavior of two-dimensional materials. Additionally, Bader *et al.*[31] proposed a double-layer graphene multi-band THz metamaterial absorber based on a Penrose tiling structure, as shown in Fig. 2. Through geometric design and material tuning, they achieved broadband, highly tunable absorption characteristics. Zhu *et al.*[32] proposed a periodic metamaterial structure consisting of three graphene strips and four C-shaped graphene square rings. By utilizing the plasmon-induced transparency (PIT) effect and the dynamic tunability of the graphene Fermi level, they

achieved broadband PIT effects and polarization angle tunability ranging from single- to triple-PIT. These works provide new insights for the design of multifunctional optoelectronic devices in the THz band.

Topological insulators, as novel quantum materials with unique electronic states, can be classified into three main types: quantum Hall (QH),[33] quantum spin Hall (QSH),[34] and quantum valley Hall (QVH)[35] metamaterials. Through low-loss surface plasmon polaritons (SPPs), high-k mode propagation, and dynamic tunability, they offer many new insights for the design and performance optimization of THz metamaterials. For example, Wang *et al.*[36] proposed a THz Dirac hyperbolic metamaterial based on topological insulators (TI), overcoming the material limitations of traditional hyperbolic metamaterials in the THz band. This structure supports up to three high-wavevector volumetric plasmonic polaritons (VPP) modes in the 5–9 THz range, with mode indices exceeding 100 and quality factors ranging from 2.19 to 6.7, outperforming traditional metal- and semiconductor-based metamaterials. Wang *et al.*[37] proposed a THz-stable topological metamaterial based on density-independent plasmons (DIPs), in which the wavelength (λ_p) of the DIPs can reach 1/66 of the free-space wavelength (λ_0), and in the 3–10 THz range, the lifetime (τ_p) of the DIPs reaches tens of picoseconds, with a Q-factor as high as 67, as shown in Fig. 3. This addresses the spectral instability issue in traditional THz plasmons caused by carrier density sensitivity.

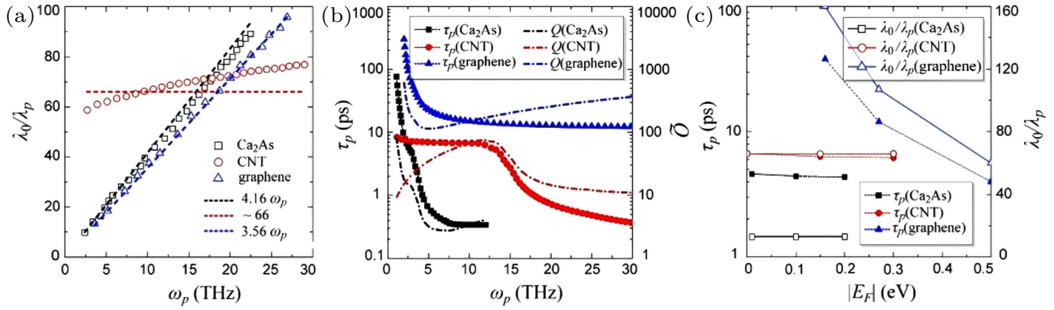


Fig. 3. Spatial constraints and lifetime of DIPs.[37]

In addition to their physical complexity, THz metamaterials also face significant challenges during the fabrication process. Since the dimensions of metamaterial units are close to or below the limits of fabrication resolution, even minor structural deviations can lead to shifts in resonance frequencies, degradation of absorption peaks, or functional failure. As a result, fabrication errors are no longer merely a secondary issue following design but rather a key factor that limits the feasibility of the design space.

Although traditional lithography, electron beam etching, and focused ion beam (FIB) processing can achieve high-precision fabrication, these techniques generally suffer from complex processes, high costs, and limited capabilities for realizing three-dimensional structures. In recent years, femtosecond laser processing and 3D printing technologies have provided new avenues for realizing complex THz metamaterial structures. For example, Won *et al.*[38] proposed a high-throughput method for fabricating THz metamaterial nanoantennas based on graphene crack lithography, as shown in Fig. 4. By introducing a graphene layer onto a flexible polymer substrate and applying tensile strain to induce the formation of ordered cracks in an aluminum oxide film, combined with oxygen plasma etching and metal deposition techniques, various nanostructures — including graphene nanoslits, graphene-metal composite nanorods, and metal nanogrooves — were successfully fabricated.

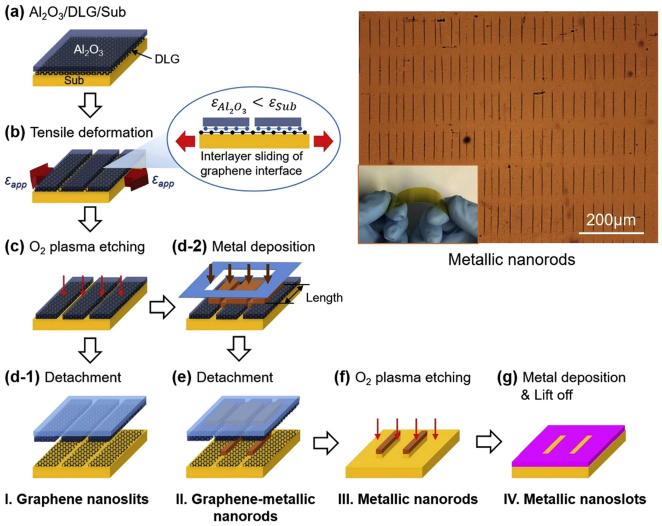


Fig. 4. Schematic diagram of graphene-based crack-lithography nanostructures.[38]

Currently, research on metamaterials has primarily focused on two-dimensional structures.[39] Although these structures exhibit extraordinary physical properties such as negative refractive index and electromagnetic invisibility, they still suffer from drawbacks such as sensitivity to the angle of incidence and difficulty in conforming to complex curved substrates, making them unsuitable for practical applications. To overcome the limitations of 2D metamaterials and expand their scope of application, researchers have turned their attention to the design and fabrication of 3D metamaterials. Technolo-

gies such as femtosecond lasers, 3D printing, and focused ion beam (FIB) processing are widely employed in this field. For example, Kim *et al.*[40] used laser printing technology to fabricate split-ring resonators (SRRs) on silicon substrates; their silver nanoparticle-based SRRs exhibited geometric dimensions and resonant responses highly consistent with those of conventional photolithographically fabricated gold SRRs. Li *et al.*[41] utilized 3D printing technology to realize an all-dielectric THz metamaterial broadband absorber, achieving an absorption rate exceeding 80% in the 0.4–1.0 THz range while maintaining transparency to visible light, demonstrating the unique advantages of 3D fabrication in functional integration. Table 1 presents a comparison of THz metamaterial fabrication technologies in recent years.

Table 1. Comparison of processing technologies.

Technology name		Processing principles	Resolution	3D capabilities	Material compatibility	Ref.
Lithography	Fabrication of free–floating metamaterials	UV/X-ray lithography + electroformed gold structure, self-supporting window frame	Micrometers ~ 10 μm	Quasi-3D (Dual-layer alignment)	Gold, SU-8 frame	[45]
	Graphene crack lithography	Utilizing the mechanical properties of bilayer graphene interfaces, combined with plasma etching and metal deposition	Submicron range ~ 100–500 nm	2.5D surface nanostructures	Graphene, metals, flexible polymers	[38]
Femtosecond laser	Two-photon polymerization (TPP)	Femtosecond laser-induced two-photon absorption cures the photopolymer only at the focal point	Submicron scale (~ 100 nm)	True 3D high-precision structure	Photosensitive polymer, requires subsequent metal plating	[44]
	Femtosecond laser-ablated metasurface	A femtosecond laser selectively removes metal layers to form an array of holes (discrete mode) or metal islands (continuous mode)	Micrometer range (~ 37–190 μm)	2D layout	Gold film, silicon substrate	[46]
3D printing	Hybrid 3D printing	FDM printing of polymer substrates, E-jet jetting of conductive materials	Micron-scale (~ 25 μm)	True 3D heterogeneous material integration	Polymer + metal composite materials	[43]
	3D-printed metal waveguides	3D-printed polymer substrate with a magnetron sputtered metal coating	Micron-scale (~ 50 μm)	Quasi-3D (Surface coating)	Polymer + metal	[42]
	FDM 3D printing	Fused deposition modeling: Layer-by-layer extrusion of thermoplastic materials	Micrometer scale (~ 100 μm)	True 3D structure	Polymers, requiring post-processing metallization	[41]

3. Core methods of algorithm-driven design

Traditional THz metamaterials can no longer meet the demands for speed, efficiency, and precision due to issues such as cumbersome simulation processes and lengthy optimization times. With the rise of artificial intelligence, algorithm-driven design and optimization of THz metamaterials have gradually come into the public eye. This paper will discuss recent advances in algorithm-driven THz metamaterial design research by examining five of the most representative algorithms: traditional optimization algorithms, machine learning, deep learning, and multi-objective optimization.

3.1. Traditional optimization algorithms

As early as the 1960s, to address the limitations of traditional analytical optimization methods — such as their tendency to get stuck in local optima and their heavy reliance on gradient information when dealing with complex nonlinear problems — John Holland of the University of Michigan, inspired by biological evolutionary processes, first systematically proposed the theoretical framework of GAs.[47,48] This method simulates the mechanisms of natural selection and genetic variation by encoding the solution to the optimization problem as "individuals." At the population level, it performs a global search through operations such as selection, crossover, and mutation, thereby gradually converging to the optimal solution without requiring explicit mathematical models or gradient information. Subsequently, in 1975, he systematically elaborated on the basic theory and methods of GAs, driving their significant development.[49] With the advancement of technology, many different optimization algorithms have been proposed, such as PSO and topology optimization. Zhang *et al.*[50] applied GA to the global optimization design of single-layer metasurface structures for the parameter optimization of broadband THz absorbers. This method combines catenary electromagnetic field theory with equivalent circuit models, significantly reducing design complexity while ensuring physical interpretability, and achieving a broadband response with an absorption rate exceeding 80% in the 1–4 THz frequency band. Through comparative validation of five typical metasurface structures, the optimized single-ring structure completed the parameter search in just 204 seconds, significantly improving design efficiency compared to traditional exhaustive design strategies driven by full-wave simulation. Wang *et al.*[51] developed a GA-based tunable vanadium dioxide (VO_2) metasurface absorber, as shown in Fig. 5. By controlling the random distribution of VO_2 pixels via 55-bit binary coding and combining it with a double-layer SiO_2 Fabry–Pérot cavity structure, they achieved a relative bandwidth of 127.8% in the 1.84–8.36 THz range. Experiments demonstrated that the VO_2 phase transition allows its electrical conductivity to be continuously tunable between 200 S/m and 200000 S/m, with the maximum absorption dynamically adjustable from 4% to

100%. Electromagnetic coupling analysis reveals that the low-frequency absorption at 2.17 THz stems from Fano resonance between VO_2 pixels, while the high-frequency absorption at 6.96 THz is dominated by Fabry–Pérot cavity resonance. Even under a 70° oblique incidence angle, the structure maintains an absorption rate exceeding 82%, breaking through the limitations of traditional sandwich absorbers in terms of bandwidth and angular stability. Anik *et al.*[52] optimized gear-shaped metamaterial structures via GA to achieve synergistic control of multiple resonance modes, obtaining triple near-perfect absorption (99.9%) in the 0.5–4.5 THz range, while also demonstrating high-sensitivity biochemical response (up to 56.67 THz/RIU), low polarization dependence (±1.2%), and excellent mechanical stability, demonstrating the significant advantages of complex structural design in multifunctional THz absorption and sensing.

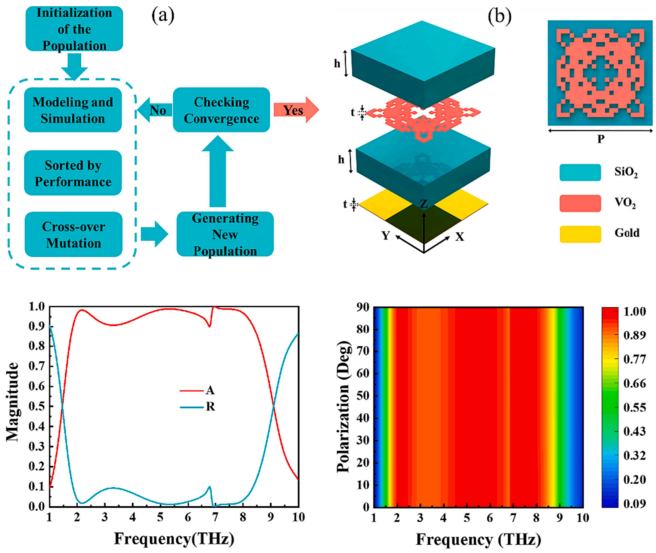


Fig. 5. (a) GA flowchart. (b) Schematic diagram of the metasurface absorber.[51]

In addition to GA, PSO is also widely used in the design of metamaterials and metasurfaces. THOMPSON *et al.*[53] used PSO to identify three potential polymer-embedded metasurface designs. By embedding silicon (Si) nanostructures into a polydimethylsiloxane (PDMS) matrix and optimizing the design using the PSO algorithm, they achieved a reflector with high reflectivity ($R \geq 99\%$) and wide spectral bandwidth ($\Delta\lambda/\lambda_0 \geq 20\%$, center wavelength$\lambda_0 = 1.55$ μm). He *et al.*[54] proposed an ultrafast all-optical THz modulation method based on inverse-designed metasurfaces. By combining the PSO algorithm with finite-difference time-domain (FDTD) simulation techniques, they designed and validated THz metasurface devices that support the electromagnetic induction transparency (EIT) effect. Li *et al.*[55] proposed a PSO-based ultra-wideband, high-efficiency metamaterial absorber. By optimizing the coupled design of multilayer planar structures and pyramid-shaped nanostructures, they achieved ultra-high performance with an average absorption rate exceeding 99.98% in the wavelength range from 300 nm to 2000 nm.

Compared to parametric geometric optimization methods, topological optimization offers greater design freedom for achieving complex electromagnetic functions by evolving material distributions within a continuous design domain. Zhou *et al.*[56] proposed a topological optimization method based on the level set algorithm, which resulted in the design of an electromagnetic metamaterial with negative permeability properties that outperforms traditional U-shaped structures in terms of negative permeability performance. This validated the effectiveness and potential of level set-based topological optimization in metamaterial design. Dong *et al.*[57] proposed a design framework for dual-negative acoustic metamaterials based on topological optimization, systematically designing, for the first time, dual-negative acoustic metamaterials based on LC resonance and Mie resonance through topological optimization. The achieved resolution reached 0.38λ. Wu *et al.*[58] employed a conjugate topological optimization method to design a free-form THz metasurface lens. By iteratively calculating gradients through forward-conjugate dual-field simulations, they evolved a 30-degree deflection device from a random initial structure in just 350 iterations. Compared to traditional phase plates with discrete prismatic structures, this continuous structure achieved a 5.5-fold increase in transmission efficiency, with a deflection efficiency of 91.3% at an operating wavelength of 2 THz. Full-wave simulations showed that the optimized electric field distribution more closely approximated a uniform plane wave, with significant suppression of higher-order diffraction. A clear deflected wavefront was formed in the *xoz* plane, providing an efficient inverse design approach for complex wavefront control devices. Saurabh *et al.*[59] investigated the influence of key parameters in topological optimization on the design and performance of two-dimensional mechanical metamaterial microstructures, aiming to achieve a bulk modulus close to the theoretical limit through parameter tuning. The results indicate that appropriate parameter selection can significantly enhance the incompressibility of the microstructure. Zeng *et al.*[60] proposed an NSGA-II-based topological inverse design method that generates a design domain-independent finite element mesh through structural variation. This approach enabled the efficient design of energy-absorbing metamaterials guided by target stress-strain criteria. Following additive manufacturing and experimental validation, the method demonstrated application potential in elastoplastic large-deformation problems and automotive passive safety.

Traditional optimization methods such as GA, PSO, and topological optimization possess strong global search capabilities in THz metamaterial design. They can effectively im-

prove design efficiency in low-to-medium-dimensional parameter spaces with well-defined objective functions, and have achieved significant results in areas such as broadband absorption, multi-frequency resonance, and wavefront control. However, in high-dimensional continuous parameter spaces and under conditions of strong nonlinearity and multi-objective constraints, these methods often face challenges such as high computational cost, limited convergence efficiency, and insufficient generalization capabilities. In particular, their heavy reliance on frequent full-wave simulation calls makes it difficult to meet the design demands of complex devices. These limitations have driven the introduction of data-driven and learning-based methods in metamaterial design, providing a crucial motivation and foundation for subsequent algorithm-driven design approaches based on machine learning and deep learning.

3.2. Machine learning-aided design

In the design of THz metamaterials, while traditional search-based optimization algorithms can identify structures that meet specific performance targets, they often suffer from limited computational efficiency and insufficient generalization capabilities when dealing with high-dimensional parameter spaces, coupled multiphysical constraints, and strongly nonlinear electromagnetic response mapping.

As a typical data-driven modeling method, machine learning can directly establish nonlinear mappings between structural parameters, material properties, and electromagnetic responses by learning from large amounts of simulation or experimental data, thereby enabling rapid forward prediction of electromagnetic performance and goal-driven inverse structural design. Compared to traditional optimization strategies, machine learning methods no longer rely on point-by-point searches but instead obtain an approximate representation of the overall structure of the design space through model training. This not only enhances design efficiency but also provides a new technical pathway for the rapid design and performance transfer of complex functional metamaterials.

Currently, machine learning-assisted THz metamaterial design primarily revolves around typical frameworks such as supervised learning, unsupervised learning, and reinforcement learning, and has already established a relatively systematic research paradigm in applications such as ultra-wideband filtering, high-sensitivity sensing, and tunable device design. Chouhan *et al.*[61] proposed a machine learning-based optimization method for the design of ultra-wideband, multi-layer stacked THz metamaterials. Forward and backward ML models were developed using ridge regression (RR), support vector regression (SVR), random forest regression (RF), neural networks (NN), and XGBoost regression. The structural parameters of an ultra-wideband band-reject filter predicted by the models with an FWHM exceeding 250 GHz, further validated the accuracy of the RF model. Finally, the RF regression model was validated by predicting ultra-wideband band-reject filters not included in the training data. Ding *et al.*[62] used the RF algorithm to design and optimize pyramid-based and inverted pyramid-based quasi-surface absorbers, as shown in Fig. 6. The results yielded a mean absolute percentage error (MAPE) of only 0.60%.

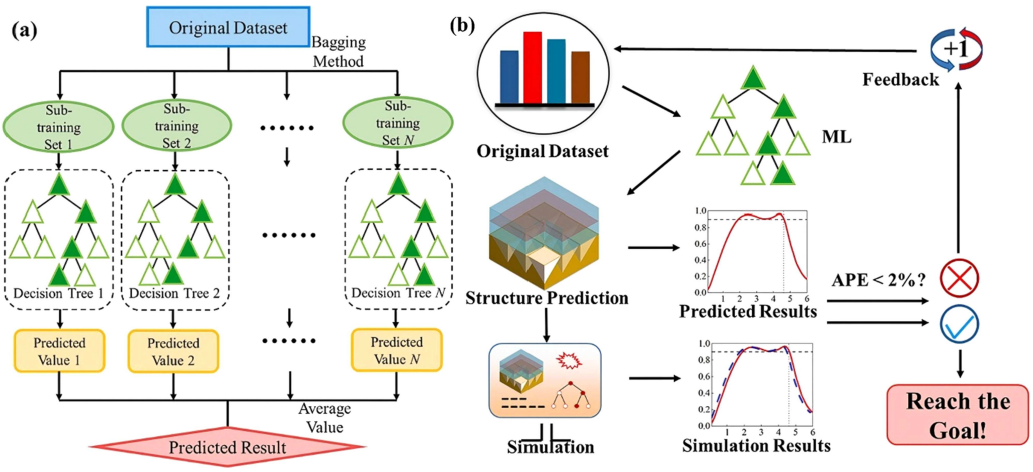


Fig. 6. (a) Schematic diagram of the RF generation process. (b) Schematic diagram of the process for predicting metasurface structural parameters using machine learning.[62]

In supervised learning, the main idea is to use labeled data to build a clear relationship between structure and response. Supervised learning is currently the most well-established paradigm in THz metamaterial machine learning research. Its core advantage lies in establishing a high-precision mapping between structural parameters and electromagnetic responses using labeled data, making it suitable for design scenarios with clear objectives and manageable data acquisition costs. Wang *et al.*[63] developed two machine learning-based models — a forward prediction model and an inverse design model — to predict the structure and optical properties of laser-fabricated gratings, as well as to determine the optimal design struc-

ture and laser processing parameters for metamaterial surfaces. The forward prediction values R^2 were 0.999 and 0.982, respectively, while in the inverse design, the two-parameter model R^2 was 0.986 and the three-parameter model R^2 was 0.878. Li *et al.*[64] proposed a machine learning-based reprogrammable metasurface imager. Sun *et al.*[65] proposed a standardized k-nearest neighbors algorithm (PS-KNN) based on polynomial regression. The mean squared error of the trained forward model was only 3.463×10^{-6}. Huang *et al.*[66] proposed a machine learning-based method for direction-of-arrival (DOA) estimation in conjunction with a tunable metasurface, by designing a 40×20 meta-atom array of a tunable transmissive metasurface, as shown in Fig. 7. Each element integrates a dual-varactor diode to achieve 235° phase control. Using a single fixed receiving probe, the system dynamically generates 24 phase patterns and combines a random forest model to directly learn the incident angle from single-point field strength data, demonstrating excellent fault tolerance (maintaining 90% accuracy even with one-third of the data missing). The system covers an incident angle range of ±60° (with a resolution of 0.1°) in the 9.5 GHz band, with a total data acquisition time of only 2.64 ms, ensuring strong real-time performance. 95.6% of estimation errors are less than 0.5°, and the average error is only 0.7°.

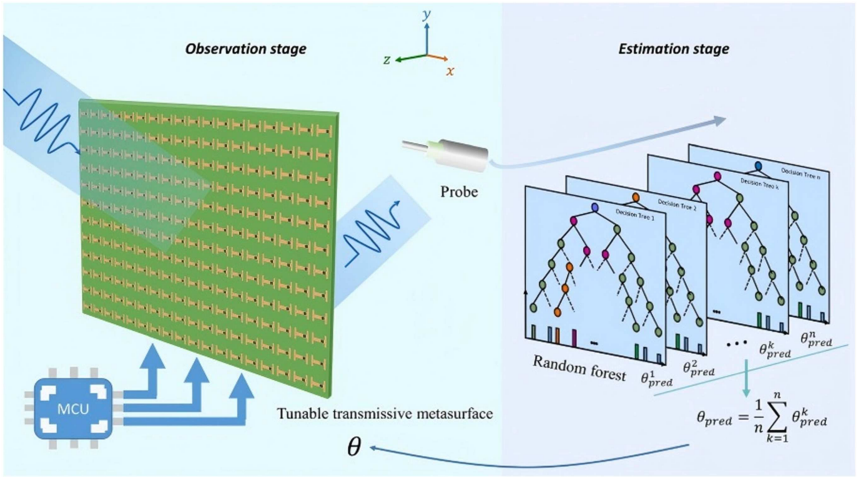


Fig. 7. Schematic diagram of a machine learning-enabled metasurface for DOA estimation.[66]

Shi *et al.*[67] proposed a machine learning-based metasurface inverse design method called artificial intelligence metasurface inverse design (AMID). Using a dataset of metasurface structures represented by 1500 randomly generated 4×4 matrices, the method employs a CNN autoencoder to perform dimensionality reduction on images of electromagnetic properties. It then uses an SVM optimized by the artificial bee colony (ABC) algorithm to map feature vectors to the metasurface structure matrix, thereby achieving classification prediction. Ultimately, AMID achieved an average classification accuracy of 81.6%, with its electromagnetic properties highly consistent with the design objectives.

Unsupervised learning, as a training and learning method in machine learning, utilizes unlabeled data to discover hidden patterns or structures within the data. Through methods such as manifold clustering and dimensionality reduction, it can help alleviate some limitations of traditional inverse design,[68] providing more flexible solutions for the intelligent design of metamaterials. Compared to supervised learning, which relies on large-scale labeled data, unsupervised learning offers greater flexibility for structure generation, multi-solution reverse engineering, and design space exploration by mining the intrinsic distribution characteristics of the data. Challapalli *et al.*[69] proposed a framework based on inverse machine learning for designing lightweight shape-memory polymer (SMP) metamaterials with record-high recovery stresses. By employing a Gaussian process regression (GPR) model and Spearman's correlation analysis, they screened for optimal structures from a vast design space, as shown in Fig. 8. Combined with fingerprinting techniques, the structures were converted into binary vectors to enable efficient processing by machine learning models. The optimized bending-dominated lattice unit achieved a 30% increase in recovery stress compared to the classical Octet lattice; the thin-walled honeycomb unit exhibited a specific recovery stress 200%–1000% higher than that of traditional honeycomb structures and 200% higher than that of solid SMP cylinders.

Reinforcement learning (RL) originated from the theory of Markov decision processes proposed in the 1960s. Its core concept involves continuously updating decision strategies through ongoing interaction between an agent and its environment, guided by a reward feedback mechanism, thereby achieving performance optimization. Unlike traditional optimization methods that rely on precise physical models, reinforcement learning can efficiently explore high-dimensional parameter spaces in the absence of prior models, offering

significant advantages in autonomous learning and dynamic decision-making. This feedback-driven learning mechanism aligns closely with the core challenges faced in THz metamaterials, particularly regarding multi-parameter strong coupling, dynamic electromagnetic response control, and design under limited data conditions. With the rapid advancement of artificial intelligence technologies, reinforcement learning has gradually emerged as a key research direction in the fields of THz metamaterial structural design and real-time control.

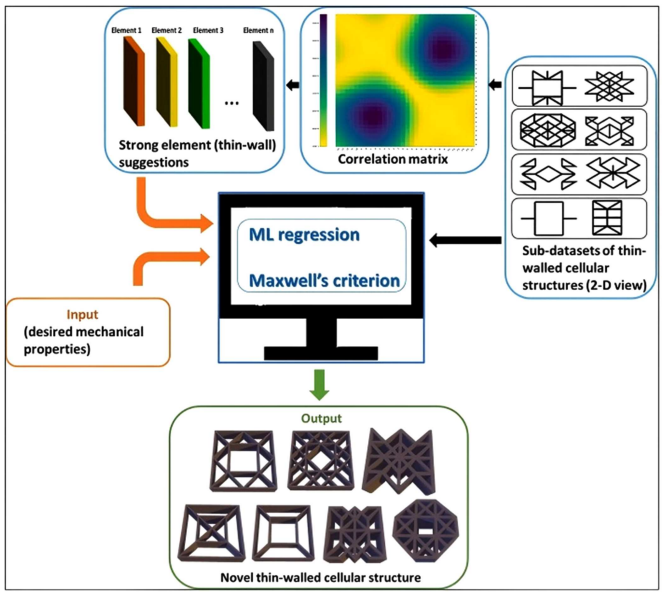


Fig. 8. Reverse design framework for optimizing thin-walled structures.[69]

Unlike supervised learning methods that rely on fixed labeled datasets, reinforcement learning continuously refines strategies through online interaction with the environment, enabling the system to achieve adaptive structural optimization or electromagnetic response control without the need for pre-constructed training labels. Therefore, this method is particularly suitable for metamaterial applications characterized by high parameter dimensions, nonlinear response behavior, and well-defined performance objectives. In practical implementation, a reinforcement learning framework typically consists of a state space, an action space, a policy network, and a reward function. Its core mechanism involves multiple rounds of policy iteration to gradually bring the metamaterial's response characteristics closer to a predefined optimal target.

In existing research, reinforcement learning has demonstrated excellent performance in tunable metamaterial systems. For example, in a study on a frequency-tunable piezoelectric metamaterial vibration system, Huang *et al.*[70] developed a reinforcement learning architecture based on the deep Q-network (DQN), enabling the algorithm to automatically adjust the parameters of the tuning circuit based on real-time vibration feedback, ultimately achieving active suppression of vibration energy across different frequency bands. This method demonstrates the potential of reinforcement learning in addressing continuous frequency modulation and structural–dynamic coupling issues. It overcomes the limitations of traditional approaches based on fixed structures or preset control models, endowing metamaterials with adaptive intelligent properties.

Compared to mechanical beamforming structures, supersurface reinforcement learning schemes for THz beam control demonstrate higher system complexity and better alignment with the design requirements of future 6G communication scenarios. For example, after Tan *et al.*[71] incorporated deep reinforcement learning into silicon-based programmable supersurfaces, the system was able to dynamically optimize beam pointing, beam spreading, and multipath compensation strategies through self-learning without the need for prior channel models. By adopting an adaptive learning mechanism based on the Actor–Critic architecture, the algorithm maintains stable beamforming performance even under conditions of extremely sparse feedback or environmental disturbances, offering significant efficiency advantages over traditional greedy search or exhaustive coding optimization methods.

Furthermore, reinforcement learning has demonstrated broad applicability in the design of optical-band structures. For example, in a recent study, Kenta *et al.*[72] utilized deep reinforcement learning to simultaneously compare three types of prediction algorithms (neural net, random forest, and XGBoost) to enhance the interpretability of geometric parameters and the reliability of optimization in the deep subwavelength structural space. This study indicates that a single algorithm may suffer from misalignment under small-sample conditions, which can easily lead to misleading structural optimization results, whereas training with a combination of multiple algorithms yields higher reliability in structural search and greater consistency in performance convergence. Furthermore, the metamaterial structures optimized via reinforcement learning achieved approximately a fivefold increase in energy harvesting efficiency, further demonstrating the performance advantages and engineering feasibility of reinforcement learning in cross-band, multi-objective metamaterial optimization.

The introduction of reinforcement learning is driving the evolution of metamaterial research from the traditional paradigm of static structural design toward a phase of intelligent control and adaptive optimization driven by environmental feedback. However, this field still faces several challenges, including a significant increase in the complexity of the learning space due to high-dimensional structural encoding, difficulties in constructing reward functions caused by multiphysics coupling effects, and the sensitivity of the online learning process to the response speed and noise levels of experimental systems. Future research is expected to reduce exploration costs by introducing model-accelerated reinforce-

ment learning, enhance algorithm generalization capabilities through transfer learning, and further integrate reinforcement learning frameworks into programmable material platforms, thereby enabling real-time closed-loop electromagnetic intelligent control for practical applications.

3.3. Deep learning and generative models

Although traditional machine learning methods can establish a mapping relationship between structural design parameters and electromagnetic responses to a certain extent, they still face significant limitations when dealing with ultra-high-dimensional design spaces, characterizing strongly nonlinear electromagnetic behavior, and generating novel structural configurations. With the advancement of deep learning technologies, their advantages in automatic feature extraction and complex mapping modeling have provided new approaches to addressing these issues. In particular, generative models such as generative adversarial networks (GANs) and variational autoencoders (VAEs) can learn underlying data distributions to actively explore potential high-performance structures within large-scale design spaces. For instance, Zhang *et al.*[73] proposed an adaptive inverse design strategy that fully leverages unsupervised GANs to achieve the intelligent design of metamaterial structures exhibiting the EIT phenomenon. Similarly, Naseri *et al.*[74] developed a deep generative design framework based on a VAE, in which both structural parameters and scattering responses were mapped into a latent space. With a jointly trained predictor network, the model ensured smoothness and physical consistency in the latent space, enabling efficient multi-objective inverse design with improved accuracy–efficiency trade-offs. This drives the transition of THz metamaterial design from traditional parameter optimization to a structure generation paradigm, significantly enhancing the flexibility and innovation capabilities of inverse design.

Beyond generative models, deep learning has also been widely applied in predictive modeling and inverse design through discriminative architectures such as convolutional neural networks (CNNs), deep neural networks (DNNs), and Transformer-based models. For instance, Yin *et al.*[75] designed an ERT model and a VAN model, as shown in Fig. 9. The former is used for forward prediction and consists of fully connected layers. It employs deep learning techniques to perform convolutional high-dimensional feature mapping on structural parameter data, stacks neural network layers via residual modules, and learns data features by combining multi-head attention mechanisms, positional encoding, and global information embedding. The latter is used for inverse design and primarily comprises convolutional layers. By leveraging the large model capacity to map data into a high-dimensional feature space for enhanced feature extraction, and employing deep convolutional techniques for efficient feature mapping, this approach also offers the advantages of few parameters and low computational complexity. Li *et al.*[76] utilized the electromagnetic properties of water and graphene in the THz band and combined them with a DNN to propose a temperature-insensitive ultra-wideband THz metamaterial absorber, achieving an absorption rate exceeding 90% in the 3.832–9 THz frequency band. The bandwidth and absorption performance can be flexibly controlled by adjusting the graphene Fermi level. Yu *et al.*[77] designed a DL-driven THz metamaterial sensor that achieves high-precision concentration prediction of anthocyanins and tannic acid in red wine (R^2 values of 0.9982 and 0.9736, respectively) by optimizing substrate thickness, metal thickness, and ring width. Furthermore, by combining resonance peak descriptors with a fully connected neural network, they achieved efficient identification of six varieties, with accuracy and F1 scores reaching 90.74% and 90.83%, respectively.

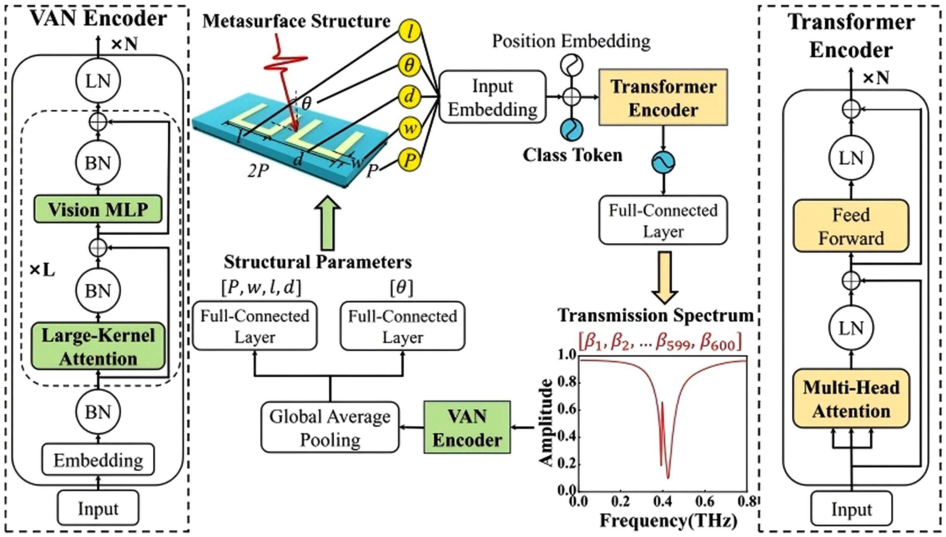


Fig. 9. Schematic diagram of the workflow for forward prediction and backward design networks.[75]

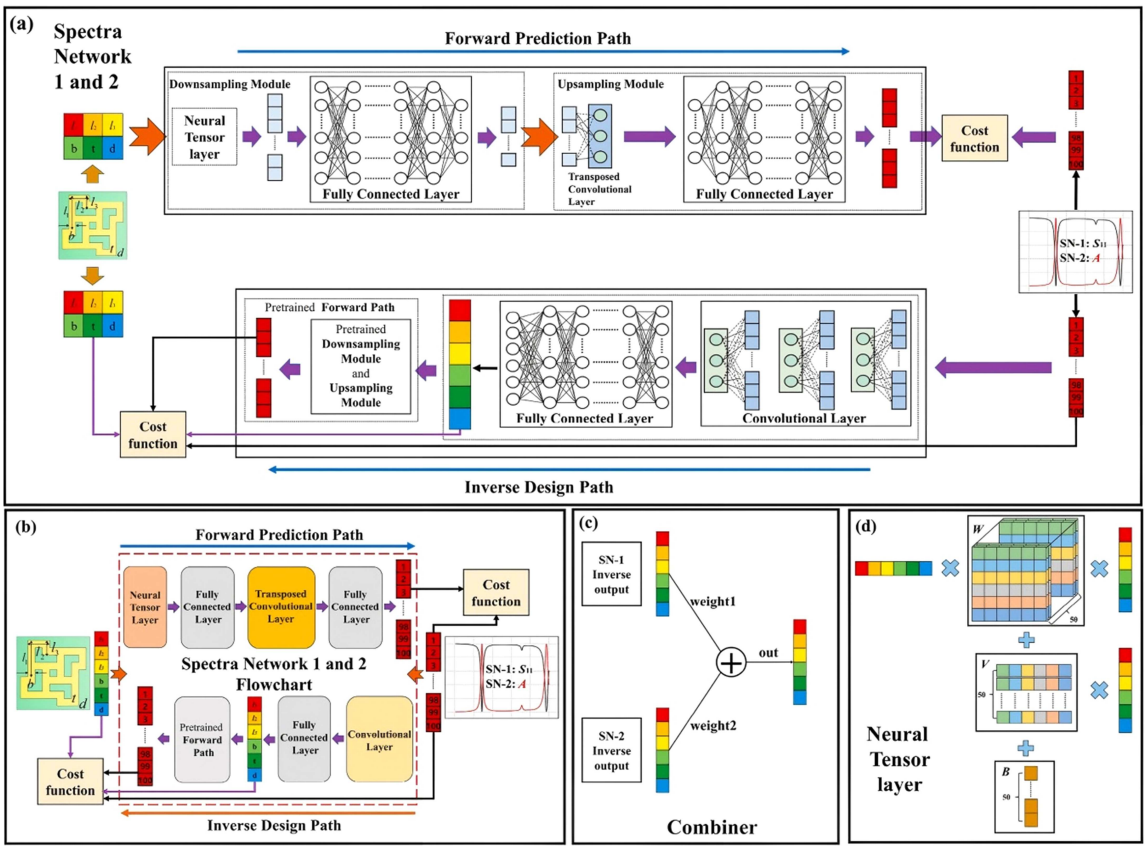


Fig. 10. Deep learning frameworks.[78]

In addition, Luo *et al.*[78] introduced a deep learning framework comprising two bidirectional spectral networks and constructed a dataset based on the intrinsic physical mechanisms of multiband THz absorbers, as shown in Fig. 10. The reflection coefficients and absorption rates of electromagnetic metamaterials in the THz range were predicted using known structural parameters. By utilizing a reverse path to generate structural parameters from the target absorption spectrum and combining the results with a weighted combiner, the framework supports the customized design of structures with two to four absorption peaks. This framework establishes a bidirectional mapping relationship between structural parameters and electromagnetic responses, demonstrating the advantages of low complexity and scalability. Cai *et al.*[79] employed a network based on the self-attention mechanism (Transformer) to achieve the inverse design of tunable broadband reflectors, demonstrating superior convergence speed and prediction accuracy compared to traditional MLP and CNN models. Ding *et al.*[80] proposed an artificial neural network (ANN)-based inverse design method to achieve ultra-wideband absorption in the 3.115–9.161 THz frequency band for a twisted bilayer graphene metasurface absorber. The absorber exhibits an absorption rate exceeding 90%, a fractional bandwidth of 98.5%, and a thickness of only 8.45 μm, outperforming existing multilayer graphene absorbers. Teng *et al.*[81] combined CNNs with GAs to achieve forward prediction and inverse design of THz random metamaterial microstructures, constructed a highly efficient encoded metasurface array, and verified its multi-beam splitting performance.

Deep learning and generative models have demonstrated significant advantages in the design of THz metamaterials: from the control of high-Q characteristics and rapid inverse design of broadband reflectors, to overcoming bottlenecks in ultra-wideband absorption performance, and the development of efficient beam splitters by combining convolutional neural networks with optimization algorithms, these methods not only significantly shorten the traditional parameter optimization cycle but also support complex functionalities such as multi-band customization, temperature insensitivity, and low polarization dependence. They achieve a high-precision mapping between target performance and structural parameters, thereby avoiding the trial-and-error nature of traditional methods. Although there is still room for improvement in multi-physics coupling modeling of 3D heterogeneous integrated structures and the generalization capability of materials with small sample sizes, these technologies have provided a solid foundation for the deep integration of multi-objective optimization strategies and automated design workflows, enabling THz metamaterial design to transition from single-performance optimization to intelligent control across the entire process under multiple constraints. Recent studies further suggest that the interaction between artificial in-

telligence and metamaterials is not unidirectional: while deep learning accelerates the design and optimization of metamaterials, these structures can also be engineered to perform physical neural computing tasks, thereby enabling hardware-level acceleration of AI algorithms. This development represents a profound integration of electromagnetic structures and intelligent computing systems, allowing algorithm-driven design paradigms to transcend the limitations of traditional optimization approaches.[82]

3.4. Multi-objective optimization and automated workflows

Although the aforementioned optimization algorithms have significantly improved the efficiency of single-objective design, practical THz devices often need to simultaneously meet multiple competing performance criteria, such as high absorption, wide bandwidth, and polarization insensitivity. In this context, a single optimal solution is no longer sufficient to meet application requirements; the design process must seek a set of optimally balanced design solutions that strike a balance among multiple performance criteria. Multi-objective optimization (MOO) algorithms have emerged as effective tools in this context. By tightly integrating optimization algorithms with manufacturing constraints and physical simulations, an automated closed-loop workflow that combines design, optimization, and verification can be established. This effectively overcomes the R&D bottlenecks caused by manual tuning and iterative trial-and-error, accelerating the transition of metamaterials from laboratory research to engineering applications.

In the field of THz sensor design, Li *et al.*[83] proposed an efficient design method for THz metamaterial sensors (TMS) based on dynamic multi-objective optimization (DMO). Using the DMO strategy, they successfully designed high-Q TMS with 2–5 resonance points, reducing the design cycle by 122 minutes compared to traditional methods. As shown in Fig. 11, taking a 3-resonance TMS as an example, simulation results demonstrated Q-factors of 301, 465, and 201, respectively, with refractive index sensitivities of 369, 376, and 387 GHz/RIU in the 0.9–1.7 THz range. The sensor exhibits specific "fingerprint peak" responses to analytes such as 2,4-D and thiabendazole, confirming its detection capability. This dynamic optimization method provides a new paradigm for the design of multi-objective metamaterial devices, particularly suitable for sensing scenarios requiring multiple high-Q resonant characteristics.

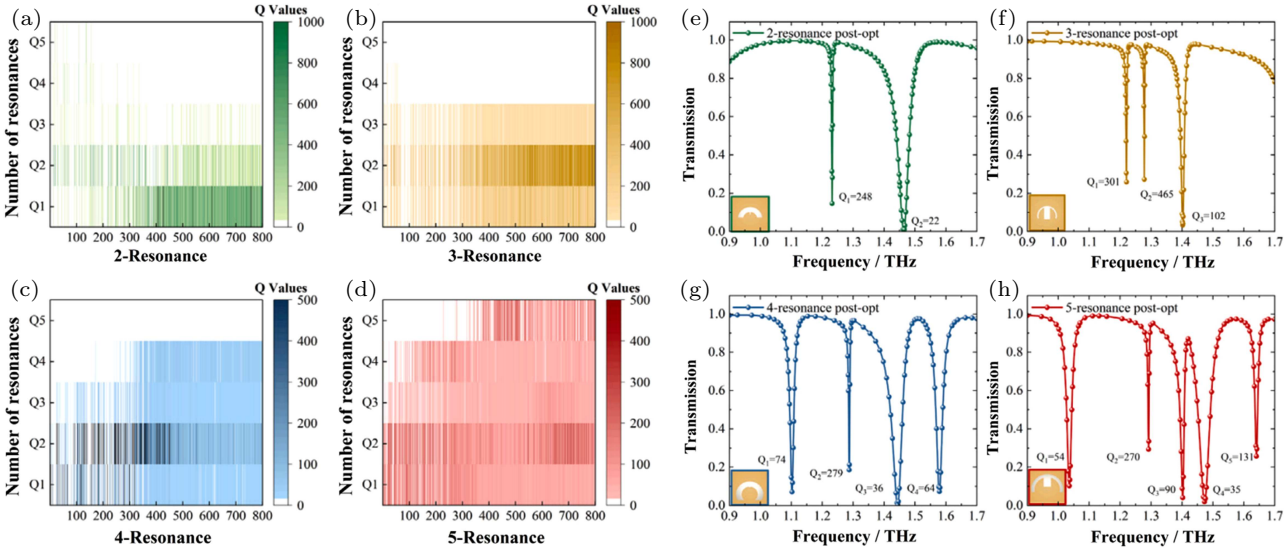


Fig. 11. (a)–(d) Q-factors of all structures during the iterative process. (e)–(h) Simulated transmission spectra of 2–5 resonance TMS at the target resonance depth and under the specified Q-factor conditions.[83]

Furthermore, to address more complex performance requirements, Ma *et al.*[84] proposed a constrained multi-objective optimization (CMOP) model to intelligently determine the optimal geometric parameters of the designed metamaterials, thereby achieving optimal multi-band absorption. In the 0.5–2 THz range, optimization using the CMOP model yielded three narrow resonance peaks with absorption values of 99.1%, 90.0%, and 99.9%, respectively. This reduced the reflection loss at the highest resonance frequency from −6.76 dB to −28.17 dB. Among these, the MA design can serve as a refractive index sensor with a maximum sensitivity of 495 GHz/RIU, a quality factor of 8.9 RIU^{-1}, a refractive index range of 1.0 to 1.6, and an analyte thickness of 18.5 μm, making it suitable for high-sensitivity liquid detection. Liu *et al.*[85] proposed a computational framework for multi-state origami metamaterials inspired by cellular automata. Complex computational tasks can be performed without the need to construct traditional logic gate networks by leveraging the physical properties of multi-state origami metamaterials. Through dynamic state transitions of stacked Miura

origami (SMO) units, nonlinear physical processes are directly applied to information processing. Experiments have verified that it can perform digit recognition, handwriting recognition, and 5-digit memory tasks using a single actuator, all meeting high accuracy requirements, thereby providing a new pathway for mechanical intelligence.

Ha *et al.*[86] proposed an automated machine learning-based inverse design process for metamaterials. By inputting user-defined stress-strain curves and 3D printing parameters, the process outputs optimal lattice design parameters, as shown in Fig. 12. The resulting 3D-printed structure achieves the target mechanical behavior. This workflow accounts for manufacturing errors and can satisfy multiple design objectives, such as adjusting stiffness and energy absorption, significantly shortening the traditional iterative cycle from design to manufacturing to final testing. Bordiga *et al.*[87] proposed a reverse-design framework for the automatic discovery of nonlinear dynamic mechanical metamaterials with reprogrammable functionality. Through gradient optimization and static pre-compression techniques, they achieved, for the first time, the automated design and functional reprogramming of nonlinear metamaterials, enabling task switching via structural deformation without the need for electronic control. Gregg *et al.*[88] proposed a self-programmable mechanical metamaterial system. Combining robotics with high-performance composite materials, the system is constructed from a 256-unit structure with a density as low as 0.0103 g/cm^3, a compressive strength of 11.38 kPa, and a stiffness of 1.1129 MPa. Based on a path planning algorithm for discrete lattice structures, it supports multi-robot collaborative operations while avoiding collisions and deadlocks. Through a distributed control architecture, it achieves efficient task allocation and incorporates fault detection and automatic recovery mechanisms. Its performance surpasses that of most comparable systems, providing a reconfigurable solution for high-performance applications such as space structures. These methods demonstrate that the synergy between multi-objective optimization strategies and automated design workflows can closely integrate algorithmic decision-making with engineering practice, ensuring that the final devices balance theoretical performance with manufacturing feasibility. This approach is gradually driving the transition of THz metamaterials from theoretical design to diverse practical applications, revealing significant application potential in critical fields such as communications, imaging, and sensing.

To facilitate a comparative analysis of the algorithmic strategies discussed above, Table 2 summarizes the representative methods, design capabilities, characteristic advantages and limitations, as well as their typical performance in THz metamaterial applications.

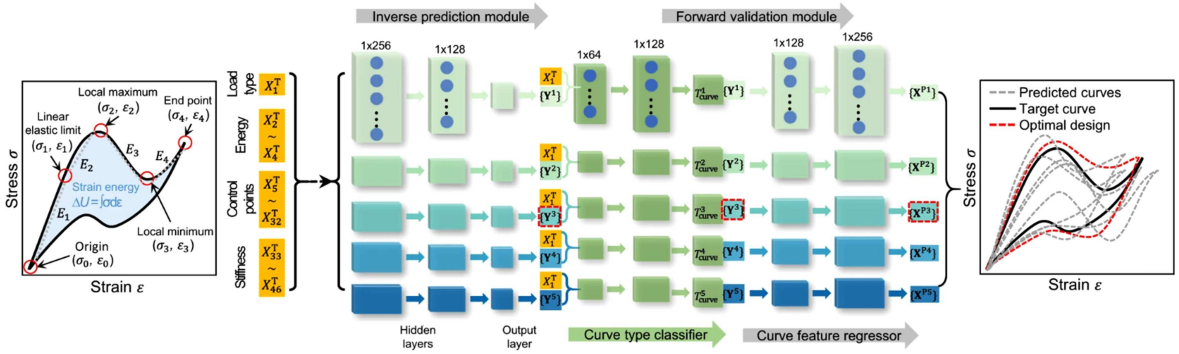


Fig. 12. Overview of a machine learning-based rapid reverse engineering method.[86]

Table 2. Comparison of algorithm-driven design methods for THz metamaterials.

Algorithm type	Representative methods	Design capability	Key characteristics	Representative performance / Applications
Traditional optimization	GA, PSO, topology optimization	Parameter optimization, structure evolution	Strong global search and physical interpretability, but computationally intensive in high-dimensional spaces	Broadband absorbers with $>$ 99.9% absorption and 127.8% relative bandwidth
Machine learning	RF, SVM, KNN, GPR	Forward prediction, inverse design	Fast surrogate prediction with reduced simulation cost, but strongly dependent on labeled datasets	DOA estimation (95.6% errors $<0.5^\circ$); metasurface prediction (MAPE = 0.60%)
Reinforcement learning	DQN, Actor–Critic	Adaptive control, dynamic optimization	Model-free adaptive optimization, but difficult reward design and unstable training	Real-time beam steering; $\sim 5\times$ energy harvesting enhancement
Deep learning	CNN, DNN, Transformer	High-dimensional mapping, image-based design	Strong nonlinear fitting and feature extraction, but data-hungry and less interpretable	Ultra-wideband absorbers ($>$ 90% absorption over 3.832–9 THz); concentration prediction ($R^2 = 0.9982$)
Generative models	GAN, VAE	Structure generation, design space exploration	Enables novel structure discovery and multi-solution inverse design, but physical constraint integration remains difficult	Multi-band metasurfaces; EIT structure generation
Multi-objective optimization	NSGA-II, DMO, CMOP	Trade-off optimization	Efficient Pareto optimization under competing objectives, but computational complexity increases rapidly	Multi-resonance THz sensors (Q-factor 465; sensitivity 495 GHz/RIU)

As summarized in Table 2, traditional optimization algorithms exhibit strong physical interpretability and global search capability, making them suitable for low-dimensional parameter optimization and structurally-constrained device design. Machine learning and deep learning methods significantly improve prediction efficiency and inverse design capability for complex electromagnetic responses, although their performance strongly depends on data quality and model generalization. In contrast, reinforcement learning and generative models demonstrate unique advantages in adaptive control and novel structure exploration, but still face challenges in training stability and physical constraint integration. Therefore, future algorithm-driven THz metamaterial design is expected to increasingly rely on hybrid frameworks that combine physical models, data-driven learning, and multi-objective optimization strategies.

4. Typical use cases for algorithm-driven systems

As algorithmic technologies continue to evolve, their applications have penetrated core areas of social production. As noted by researchers at Google,[89] the development of AI algorithms has transcended traditionally isolated disciplines; these algorithms can enhance the design and execution of scientific research and are becoming indispensable tools for researchers. This assertion has been fully validated by industrial practice in recent years. The algorithm-driven model is transitioning from laboratory prototypes to large-scale deployment, and in this process, collaborative innovation between academia and industry has played a pivotal role.

In recent years, the design of functional devices in the THz band has undergone a paradigm shift. Intelligent algorithms, exemplified by deep learning, have not only significantly improved design efficiency but also expanded the boundaries of traditional optimization methods. For example, Huang *et al.*[90] proposed a method for the inverse design of multi-resonant graphene metasurfaces based on an improved Transformer and a conditional generative adversarial network. This method demonstrates good predictive capability in mapping spectral and structural parameters and can directly generate structural images, thereby enhancing the intuitiveness and stability of the design process. The designed multi-resonant metasurface structure is suitable for applications such as multi-frequency THz modulation and filtering, and holds practical significance for communication devices that need to simultaneously meet multiple operating frequencies. Researchers Zhang *et al.*[91] developed an automatic inverse design framework for dual-metasurface THz absorbers by integrating genetic algorithms (GA) with catenary field theory. This method achieves broadband impedance matching by optimizing the dispersion distribution and can output optimal structural parameters in just 10–20 seconds. The designed absorber exhibits an absorption rate exceeding 88% within the 0.21–5 THz bandwidth and can flexibly achieve low-pass filtering characteristics by adjusting the objective function. These algorithm-driven THz metamaterial design methods not only enhance design efficiency and device performance but also significantly broaden their application scope.

In the field of chemical and biological detection, THz radiation is highly sensitive to weak intermolecular interactions; however, the weak absorption signals from target molecules and susceptibility to environmental interference limit the detection performance of traditionally designed devices. Recent advances have shown that material-driven enhancement strategies, including metamaterials, two-dimensional materials, and hybrid systems, can significantly improve sensing performance by enabling local field enhancement, dynamic resonance tuning, and molecular-specific interactions.[92] In recent years, algorithm-driven metamaterial design and data analysis methods have provided effective solutions to this problem, enabling THz chemical detection to gradually evolve from structural enhancement toward intelligent sensing. At the device level, algorithmic models are employed for the inverse design of multi-resonant metamaterial structures to enhance the characteristic response of target molecules, thereby improving the detection sensitivity for trace substances. For example, Abdullah *et al.*[93] proposed a machine learning-assisted design method for THz metasurface chemical sensors, utilizing models such as random forest regression to model and predict the relationship between structural parameters and performance. This approach achieved highly sensitive chemical detection while significantly reducing design and simulation costs, demonstrating excellent detection performance in complex chemical environments. Yang *et al.*[94] proposed a pesticide detection method combining THz metamaterial sensors with machine learning models. By enhancing molecular fingerprint signals through resonant structure design and utilizing regression algorithms, they achieved highly sensitive quantitative identification of carbendazim concentrations, demonstrating that algorithm-assisted structural design and signal modeling can effectively overcome the limitations of traditional single-threshold detection. At the data level, the role of algorithms in THz chemical detection has been further expanded from structural optimization to the core of spectral analysis and intelligent recognition.

In addition to structural design, algorithmic models also play an important role in spectral analysis and intelligent recognition. Yu *et al.*[95] introduced stacked long short-term memory (SLSTM) networks into THz spectral analysis. By treating continuous spectra as sequence data to learn their long-range correlations and combining this with the permutation significance method to screen for key frequency bands,

they achieved rapid identification of complex biochemical systems. Furthermore, data fusion strategies have been introduced to improve multi-target detection capability. Li *et al.*[96] constructed a machine learning-enhanced flexible metamaterial biosensing platform, achieving both qualitative and quantitative detection of various pesticides and effectively mitigating spectral overlap issues. The multi-response variable competitive selection fusion (MRR-CSF) framework proposed by Zhang *et al.*[97] significantly improved the accuracy and robustness of trace antibiotic detection by fusing response variables such as multi-wavelength resonance peak intensity and peak area. The detection limit was as low as 5 ng/L, with a 12%–27% improvement in accuracy compared to single-variable regression models.

In THz communication systems, stringent requirements are placed on the selectivity, stability, and manufacturability of filters. To address these needs, Ju *et al.*[98] employed DBS and BPSO algorithms to perform the inverse design of a pixelated THz bandpass filter, and experimentally verified the device performance using femtosecond laser processing and a THz time-domain spectroscopy system. This method achieved a well-balanced performance in terms of peak transmittance, out-of-band rejection, operating bandwidth, and polarization stability, demonstrating that intelligent algorithms are well-suited for the design of complex communication devices. Meanwhile, in the field of quantum communication, to address the technical requirements for simulating quantum algorithms in the THz band, Blackwell *et al.*[99] designed an all-dielectric metastructure quantum algorithm simulator comprising silicon-based qubit sub-blocks and Kapton polyimide gradient refractive index (GRIN) lenses. Following preliminary optimization through numerical analysis, machine learning-driven inverse design was employed to further enhance the device's simulation performance for the Deutsch–Jozsa algorithm. This method provides critical support for the field of quantum communication.

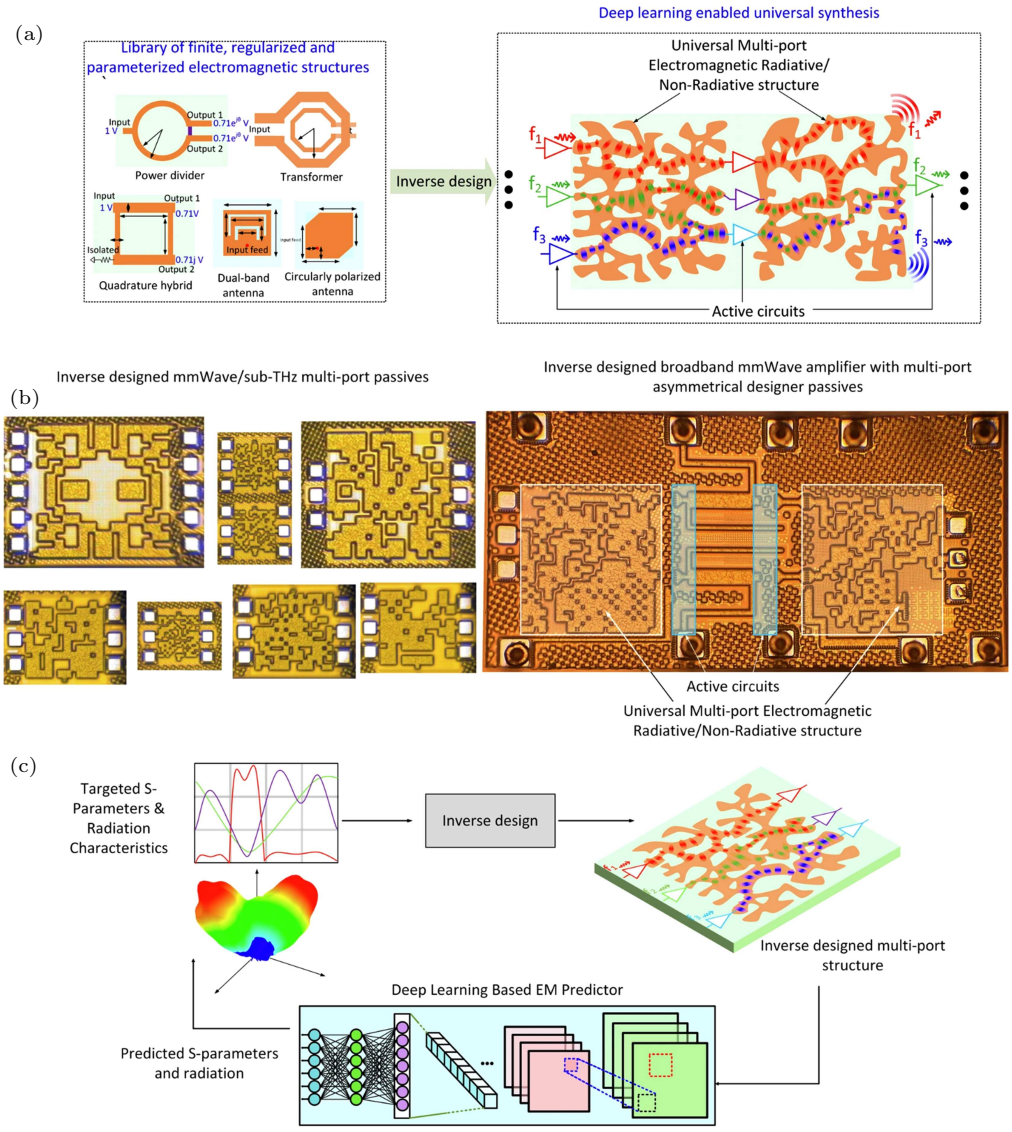


Fig. 13. A general-purpose circuit for the inverse synthesis of high-frequency signals using deep learning.[103]

In addition, the application of these algorithms has expanded from the optimization of individual devices to multiple critical components of THz communication systems. In the areas of filtering and spectrum shaping, Yu *et al.*[100] used a genetic algorithm (GA) to simultaneously optimize the filter's transmission, out-of-band rejection, and structural manufacturability, resulting in a THz metasurface filter with excellent selectivity and stability, thereby demonstrating the reliability of evolutionary algorithms in the design of complex communication devices. To address the needs of beam control and spatial multiplexing, Fakharian *et al.*[101] proposed a machine learning-based metasurface inverse design method capable of rapidly generating multi-beam THz coding metasurfaces, reducing side lobe levels, and improving beamforming accuracy, thereby providing a new approach for high-capacity THz wireless communications. In dynamic communication scenarios, Fan *et al.*[102] applied deep reinforcement learning to reconfigurable THz metasurfaces, enabling real-time beam scanning and link-adaptive adjustment without the need for precise physical models, thereby demonstrating the algorithm's advantages in complex channel environments. In the field of antenna design, Karahan *et al.*[103] proposed a deep learning-driven universal inverse design framework, as shown in Fig. 13. It systematically demonstrates how the algorithm can directly generate structures for multi-port RF and sub-THz passive devices. This method takes target scattering parameters as input and uses neural networks to search for optimal topological structures in high-dimensional geometric space that satisfy multi-port coupling and impedance matching requirements, thereby achieving unified inverse design for filters, power dividers, and integrated circuit passive modules. Additionally, Hu *et al.*[104] developed a machine learning surrogate model for the rapid design and performance prediction of THz metasurface modulators, achieving joint control of amplitude and phase, and providing a viable device solution for high-bit-rate THz communication systems. In summary, algorithms play a pivotal role in the design of THz metamaterials and metasurfaces, transforming the approach to R&D for THz communication devices. The traditional static parameter optimization has evolved into intelligent design and adaptive tuning focused on system performance, providing crucial technical support for future high-capacity, low-latency, and highly reliable THz communication systems.

In the field of biosensing, algorithm-assisted THz metamaterials further extend their capabilities to complex biological environments, where both high sensitivity and specificity are required. Algorithm-aided THz metamaterials have been widely employed to enhance sensing performance and enable accurate analyte identification through data-driven modeling and optimization strategies.[105,106] As a representative example, the graphene-based metasurface shown in Fig. 14 demonstrates ultra-wideband molecular fingerprint sensing, where an inversion algorithm is introduced to reconstruct distorted spectral responses and achieve high-fidelity identification of trace analytes.[107]

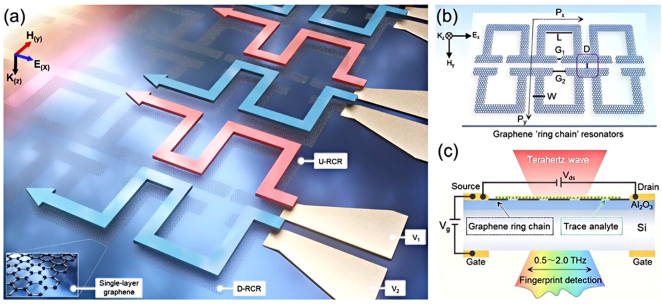


Fig. 14. Design concept of the proposed reconfigurable graphene metasurface.[107]

At the device design level, algorithmic models are used to achieve the precise design of metamaterial structures with multiple resonances and high selectivity, providing a foundation for weak signal amplification. By exploring the nonlinear relationship between structural parameters and electromagnetic responses, these algorithms overcome the limitations of empirical design and efficiently generate structural configurations that match the characteristics of biomolecules. Hu *et al.*[108] proposed a machine-learning-assisted peptide/MXene composite metamaterial sensor array. By optimizing peptide selection and loading methods through algorithms, the sensors achieved a response to target gases approximately 150% higher than that of pure MXene. Furthermore, by combining feature dimensionality reduction and classification algorithms, they achieved accurate identification of various cancer-related VOCs. Zamzam *et al.*[109] utilized deep learning to optimize graphene metamaterial structures, achieving polarization-insensitive near-total absorption devices. Furthermore, by analyzing tissue spectra via neural networks, they achieved high recognition accuracy in breast cancer tissue detection, demonstrating the advantages of synergistic optimization between structural design and data analysis. Zhang *et al.*[110] proposed a reverse-design framework based on data-driven iterative strategies and conditional variational autoencoders, significantly increasing the proportion of strongly circularly dichroic structures in the design space and providing a customizable device solution for the detection of chiral biomolecules. At the data processing level, algorithms have become key tools for THz spectral analysis and biosignal recognition. To address the challenges of high-dimensional and noisy spectra in biological samples, researchers commonly employ dimension reduction, feature selection, and classification algorithms to enhance detection reliability.

In addition, machine learning algorithms have been widely used for feature extraction and classification of complex biological spectra, improving robustness under noisy and

high-dimensional conditions. Zhu *et al.*[111] introduced machine learning methods into a plasma-enhanced infrared spectroscopy system, achieving rapid quantification of disease biomarkers such as acetone at sub-ppm concentrations, significantly reducing the impact of cross-interference, and validating the algorithm's effectiveness in weak feature extraction. At the multimodal application level, algorithm-driven metamaterial platforms have achieved the integration of sensing and imaging functions to meet the diverse needs of clinical diagnosis. Beyond sensing tasks, algorithm-driven THz metamaterials have also shown strong potential in imaging and non-destructive analysis. Kim *et al.*[112] designed a frequency-tunable THz metamaterial chip that, combined with differential signal processing algorithms, enabled cell type identification and dynamic monitoring of the microenvironment. Liao *et al.*[113] designed a multi-resonant metamaterial array based on quasi-bound-state dispersion engineering and, in conjunction with compressed sensing algorithms, achieved high-speed single-pixel imaging, outperforming traditional THz systems in both spectral resolution and imaging speed. Mohammadiaria *et al.*[114] further proposed algorithmically controlled reconfigurable metasurfaces that tune resonant characteristics and wavefront distributions in real time, providing better system adaptability for bioelectronic implantable devices.

Overall, the role of algorithms in the biological applications of THz metamaterials has evolved from a simple structural optimization tool to a core method that spans device design, signal analysis, and functional implementation. By using inverse design to enhance device response specificity, machine learning to extract subtle features, and multi-algorithm collaboration to achieve multimodal sensing, algorithm-driven THz metamaterials show great promise in applications such as non-invasive cancer detection, analysis of the cellular microenvironment, and high-resolution biological imaging. As algorithms and metamaterial technology continue to converge, this field is expected to play an increasingly significant role in early disease diagnosis and personalized medicine.

5. Challenges and future directions

5.1. Current challenges

Against the backdrop of algorithm-driven design gradually being introduced into THz metamaterial research, multi-target detection and dynamic control have emerged as key areas of development. As the number of detection targets increases and operating environments become more complex, devices face new constraints in structural design, model development, and system implementation. Existing methods still have shortcomings in terms of resonant degrees of freedom, computational efficiency, and system integration capabilities, making it difficult to fully meet practical requirements under multi-target conditions. Therefore, it is necessary to systematically examine and analyze the challenges faced in current research across three levels: physical mechanisms, algorithmic methods, and system integration.

At the level of physical mechanisms, the transition from single-layer structures to multi-layer structures and multimodal mechanisms represents a key direction for overcoming the limitations of multi-target detection. During actual dynamic control processes, metamaterials are typically subjected to multiple physical forces — including electromagnetic, thermal, and mechanical forces — simultaneously, resulting in response characteristics that are distinctly nonlinear and time-varying. However, single-layer structures offer limited resonant degrees of freedom, making it easy for response signals corresponding to different targets to overlap or interfere with one another. When multiple targets act simultaneously on the device surface, cross-effects may also arise between different perturbations through electromagnetic coupling, making response analysis even more challenging. Currently, most simulation and design methods are still based on single-physics-field or weak-coupling assumptions, making it difficult to accurately describe the actual operating state under multi-target conditions, a limitation that is particularly evident in complex environments.

At the algorithmic level, building high-performance models and enhancing computational capabilities are critical to addressing the complexity of multi-objective design. The deep integration of artificial intelligence and metamaterials will continue to drive the evolution of design methodologies. Forward prediction models can significantly reduce the computation time for electromagnetic responses, while generative inverse design methods help construct a richer structural solution space, thereby accommodating multi-objective and multi-constraint requirements. At the same time, incorporating fundamental electromagnetic equations and material constitutive relations into the model training process can, to some extent, reduce reliance on large-scale data while improving model stability and interpretability. With advancements in computational power, the efficiency of multi-objective optimization and high-dimensional parameter search is expected to improve. Furthermore, integrating real-time sensing and reinforcement learning to build closed-loop systems will provide a technical foundation for dynamic control and adaptive detection.

At the system integration level, achieving integration and intelligence is a necessary path for THz metamaterials to transition from experimental research to practical applications. Through cross-scale collaborative design, the integrated integration of modulation units, detection units, and control modules helps improve overall performance while reducing system size. In specific applications, highly sensitive sensing structures for biomedical detection, as well as low-loss transmission and control devices for communication scenarios, have already demonstrated initial application potential. Further integration of programmable metamaterials with intelligent al-

gorithms to enable real-time adjustment of THz spectral and spatial responses is expected to support complex requirements such as multi-band communication and multi-target detection. Currently, such systems remain in the early stages of application, and future research must continue to focus on issues of compatibility, stability, and long-term reliability across different levels of integration.

Despite the rapid progress of artificial intelligence in THz metamaterial design, the limited interpretability of data-driven models remains a major unresolved scientific challenge. Most artificial intelligence methods serve as black-box models, where the complex mapping between structural parameters and electromagnetic responses lacks explicit physical interpretation, particularly under strongly nonlinear and multiphysics-coupled conditions. Although existing models can achieve high prediction accuracy and efficient inverse design, their limited physical interpretability restricts deeper understanding of the underlying electromagnetic mechanisms and reduces model reliability beyond the training space. Potential solutions include incorporating physical priors and constraints into model architectures, developing physics-informed learning frameworks, and combining data-driven models with analytical or semi-analytical approaches. These strategies aim to bridge the gap between predictive performance and physical understanding, enabling algorithm-driven design to evolve from a purely optimization tool toward a framework with improved physical interpretability.

5.2. Future trends

In light of the aforementioned challenges, and based on the preceding analysis of structural design, algorithmic methods, and engineering implementation, it is evident that algorithm-driven research on THz metamaterials is gradually shifting from the optimization of individual properties toward system-level design tailored to complex environments and multi-objective requirements. Future development efforts will focus not on pushing individual metrics to their absolute limits, but rather on achieving stable performance, structural controllability, and system usability under real-world application conditions.

At the level of physical mechanisms and structural design, the transition from single-layer metamaterials to multi-layer structures and multi-degree-of-freedom control represents a direct approach to addressing the demands of multi-target detection. Existing devices are mostly based on single-layer resonant structures, which have limited operating bandwidth and distinguishable response channels, making them prone to signal coupling and response aliasing when multiple targets act simultaneously. By introducing multilayer structures or multimodal coupling mechanisms, independent response channels can be added in the spatial or frequency dimensions, thereby improving the ability to distinguish between different targets. At the same time, mechanisms discussed earlier — such as the electromagnetically induced transparency effect and continuum bound states — provide effective means to enhance the quality factor and response sensitivity within finite structural dimensions. While these methods enhance sensing performance, they also impose higher demands on structural precision and fabrication, and their engineering implementation requires further research.

At the algorithm and model level, improving model performance and enhancing computational capabilities are essential prerequisites for supporting high-dimensional, multi-objective design. As noted earlier, deep learning-driven inverse design methods still have shortcomings in terms of data efficiency and generalization ability, and multi-objective detection further exacerbates this issue. Future research should build upon existing forward prediction and generative design frameworks by incorporating physical constraints and multi-objective optimization strategies to reduce reliance on large-scale data and improve model stability under complex conditions. At the same time, as the number of parameters and optimization objectives increases, the demand for computational power and algorithmic efficiency will continue to rise. By integrating reinforcement learning and closed-loop optimization approaches, it is expected that faster responses and adaptive adjustments can be achieved in dynamic control scenarios, providing algorithmic support for programmable metamaterials and real-time control devices.

At the system implementation and application levels, achieving integration and intelligence is a necessary step for THz metamaterials to move toward practical applications. As analyzed earlier, most current research remains at the device-level verification stage, with systems relying on external control and signal processing modules, resulting in relatively high overall complexity. In the future, cross-scale integration will be required to integrate modulation, detection, and control functions into a unified design, thereby reducing system size and improving response speed. Building on this foundation, combining programmable metamaterials with intelligent algorithms will enable dynamic reconfiguration of THz responses, supporting the fusion of multi-objective detection and communication sensing. Although related research is still in the early stages of application, it has already demonstrated preliminary feasibility in areas such as communications, biosensing, and imaging.

Within the aforementioned framework of collaborative development, as algorithms are gradually integrated into THz metamaterial research, it remains essential to strike a balance between their physical fundamentals and the freedom of structural design. Although data-driven methods demonstrate clear advantages in accelerating structural optimization and performance prediction, overreliance on metric-driven model training may, to some extent, limit the scope for exploring novel physical mechanisms and unconventional structures. Looking

back at the development of metamaterials, many key advancements did not stem directly from the optimization of predetermined objectives, but rather from the observation of anomalous phenomena and the understanding of underlying physical mechanisms. Such breakthroughs are often difficult to fully replicate using existing deep learning frameworks. Therefore, a more promising research path lies in guiding intelligent algorithms to deepen their understanding of the physics of sensors, rather than merely pursuing the extreme optimization of performance metrics. In this process, numerous issues regarding the deep synergy among physical mechanisms, algorithmic models, and engineering implementation remain to be explored. Gradual breakthroughs in these areas are expected to drive the evolution of THz metamaterials toward practical applications in a more robust and sustainable manner.

6. Conclusions

Algorithm-driven design has become the core driving force behind the shift in THz metamaterials from an empirical approach to systematic and intelligent design. Compared to traditional design methods that rely on parameter scanning and human experience, data-driven and intelligent optimization methods have redefined the mapping relationships among structural parameters, material properties, and electromagnetic responses, transforming the design of complex functional devices from an inefficient trial-and-error process to a predictable and controllable rational approach. The introduction of multi-objective optimization, machine learning, and deep generative models has not only significantly shortened the design cycle for high-dimensional structures but also provided new technical pathways to overcome multi-physics coupling constraints and achieve high quality factors, broadband tunability, and multifunctional integration. Through the incorporation of physical prior constraints, the stability and interpretability of algorithmic models under small-sample conditions have been enhanced, thereby enabling THz metamaterials to demonstrate performance potential that surpasses traditional methods in applications such as sensing, communications, and imaging.

In the future, the further development of THz metamaterials will depend on the establishment of a multi-physics modeling and validation framework, the in-depth optimization of intelligent algorithms, and the synergistic integration of materials, devices, and manufacturing processes. This will bridge the gap between algorithmic predictions and actual performance, enhance the generalization capabilities of models under complex structural and limited data conditions, and accelerate the transition from proof-of-concept to engineering applications. As these challenges are gradually addressed, algorithm-driven THz metamaterials are expected to play a more fundamental and enduring supporting role in various cutting-edge technological systems, achieving functional diversification, high-performance efficiency, and intelligent applications.

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