Advances in Engineering Research : Possibilities and Challenges
ISSN Print: 3079-5192
ISSN Online: 3079-5206
https://doi.org/10.63313/AERpc.9057

Data-Driven Inverse Design of THz Metamaterials: A Deep Learning Approach for Small-Data Regimes

Peng Xu
College of Engineering, Tianjin University of Technology and Education, No. 1310, Dagu South Road, Hexi District, Tianjin 300222, China
Email: 550184452@qq.com

How to cite this paper: Xu, P. (2025). Data-Driven Inverse Design of THz Metamaterials: A Deep Learning Approach for Small-Data Regimes. Advances in Engineering Research: Possibilities and Challenges, 2(3), 54-64. ISSN Print: 3079-5192; ISSN Online: 3079-5206.
https://doi.org/10.63313/AERpc.9057
Published: 2025-11-05

Abstract

Inverse design based on deep learning offers a revolutionary paradigm for ac-celerating the development of novel terahertz (THz) metamaterials. However, its application is often constrained by the high cost of acquiring large-scale sim-ulation datasets. This work focuses on the high-accuracy inverse design of THz electromagnetically induced transparency (EIT) metamaterials under small da-taset conditions, systematically evaluating the effectiveness of different deep learning architectures.

To achieve precise inversion from a target spectrum to its physical structure, we constructed a representative dataset through parametric electromagnetic si-mu-lation. On this foundation, we built, trained, and compared three neural network models: a Multi-Layer Perceptron (MLP) as the baseline, a residual fully con-nected network (FC-ResNet) for enhanced deep network training, and a one-dimensional convolutional neural network (1D-CNN) designed for sequen-tial data.

The results reveal a key finding: for this inverse design task, the FC-ResNet demonstrated superior predictive performance, achieving a coefficient of de-termination (R^2) of 0.9794 on an independent test set. This significantly out-performed the baseline MLP (0.9438) and surprisingly surpassed the theo-reti-cally more suitable 1D-CNN. Further analysis suggests that for the EIT inverse problem investigated here, the prediction relies more on the global morphology and correlation features of the spectrum than on localized characteristics. The FC-ResNet, with its deep architecture and effective residual learning mecha-nism, successfully captured this complex, non-local mapping relationship. The core contribution of this work is demonstrating that for complex physical prob-lems, a deep, general-purpose model with sufficient expressive power and stable trainability can outperform a more specialized architecture that is prone to in-formation loss. This finding provides a crucial guideline for model selection in the intelligent design of physical devices, particularly in resource-constrained scenarios

Keywords

Inverse Design; Terahertz Metamaterials; Deep Learning

1. Introduction

Within the electromagnetic spectrum, the Terahertz (THz) band (0.1-10 THz), situated between microwaves and infrared light, has long been referred to as the "THz gap" due to the historical lack of efficient sources and detectors [1]. However, with continuous technological advancements, the unique physical properties of THz waves are positioning them as a focal point for scientific research and cutting-edge applications. Their low photon energy causes no ionization damage to biological tissues, offering a distinct safety advantage in biomedical imaging. Their ability to penetrate various non-metallic, non-polar materials provides new technological pathways for non-destructive testing and security screening. Furthermore, their broad spectral resources indicate significant potential for future ultra-high-speed wireless communication [2]. Despite these promising applications, the advancement of THz technology remains constrained by a fundamental challenge: most natural materials exhibit very weak responses to THz waves, making it exceptionally difficult to fabricate functional devices that can efficiently manipulate their propagation characteristics.

To overcome this material bottleneck, metamaterials—composed of periodic arrays of subwavelength artificial structures—offer a revolutionary solution [3]. Unlike traditional materials that rely on their inherent chemical composition, the electromagnetic properties of metamaterials are primarily determined by the geometric shape, dimensions, and arrangement of their unit cells. This "design-as-material" concept allows for the flexible customization of electromagnetic wave amplitude, phase, polarization, and even transmission modes through ingenious structural design, enabling exotic electromagnetic responses—such as negative refractive index and perfect absorption—unattainable with natural materials [4]. This opens vast possibilities for developing high-performance, miniaturized THz functional devices.

Among the various physical effects realized by metamaterials, the Electromagnetically Induced Transparency (EIT) phenomenon has garnered significant attention due to its unique physical implications and application value [5, 6]. The EIT effect, achieved through the near-field coupling between a radiative ("bright") mode and a non-radiative ("dark") resonant mode within the structure, creates an exceptionally sharp transparency window within an originally broad absorption spectrum [7]. This transparency window is accompanied by strong dispersion effects and group velocity delay, making EIT metamaterials particularly promising for applications requiring precise spectral control and strong light-matter interactions, such as high-sensitivity refractive index sensors, tunable slow-light devices, and narrowband filters [8].

However, achieving an EIT window with specific performance necessitates the precise design of its microstructural parameters, which is a highly challenging task. Traditional "forward design" methodologies heavily rely on the designer's physical intuition and an iterative trial-and-error process. Researchers first conceptualize an initial structure, then use numerical electromagnetic simulation software for time-consuming simulations to analyze its spectral response. Based on the results, geometric parameters are manually adjusted, and this process is repeated until satisfactory performance is achieved. As the number of parameters requiring optimization increases, this parameter-sweeping approach faces the "curse of dimensionality," where computational costs grow exponentially. This process is not only inefficient but also highly prone to becoming trapped in local optima within the parameter space, potentially missing the global optimum.

To fundamentally transform this inefficient design paradigm, Artificial Intelligence (AI)-based "inverse design" has emerged [9, 10]. This approach reverses the design workflow: it starts from the desired performance (i.e., the target spectrum) and utilizes algorithms to directly and rapidly predict the physical structure that can achieve that performance. Deep learning, a core AI technology, has become the preferred tool for realizing efficient inverse design due to its powerful capability for modeling complex nonlinear relationships and automatically extracting features from data [10-14]. Nevertheless, the exceptional performance of deep neural networks is typically built upon massive training datasets. In the metamaterials domain, acquiring a single data sample requires a complete electromagnetic simulation, representing a significant cost in terms of computational resources and time. Therefore, a critical challenge that must be addressed to transition deep learning from theory to practical engineering applications is how to train inverse design models that maintain high accuracy and strong generalization capability under the constraint of a limited number of samples (i.e., "small dataset") [15-18].

This study aims to address the aforementioned challenge by exploring effective methods for the rapid and intelligent inverse design of THz EIT metamaterials driven by small datasets. To this end, we construct a dataset through parametric electromagnetic simulations. Based on this dataset, we systematically investigate and compare the performance of different types of deep learning models in solving this inverse problem. The focus is on evaluating basic Multi-Layer Perceptron (MLP), one-dimensional Convolutional Neural Networks (1D-CNN) optimized for sequential spectral data [19], and advanced network architectures incorporating residual learning (ResNet) mechanisms [20]. The objective of this research is to conduct an in-depth assessment of the prediction accuracy, stability, and generalization ability of these models when trained on small datasets, thereby providing a practical and efficient solution for the automated design of high-performance THz devices under resource-constrained conditions.

2. Theory and Methods

The primary objective of this study is to establish an inverse mapping model from the terahertz spectrum to the structural parameters of a metamaterial. To this end, we first designed a classic EIT metamaterial structure and utilized the commercial electromagnetic simulation software CST Studio Suite to perform full-wave numerical simulations for dataset construction. Subsequently, using the PyTorch deep learning framework, we built and trained three distinct neural network models based on this dataset to accurately predict the structural parameters from a target spectrum.

The unit cell of our designed THz EIT metamaterial is illustrated in Figure 1(a). The structure consists of a central metallic wire and two pairs of symmetrically distributed Split-Ring Resonators (SRRs), all deposited on a lossless dielectric substrate, as shown in the side view in Figure 1(b). Under normal incidence of a THz wave, the central wire acts as a "bright mode" that directly couples with the incident electric field, while the SRRs function as a "dark mode" that interferes with the bright mode through near-field coupling, thereby producing the EIT effect.

To obtain the spectral response of this structure, we conducted systematic simulations in CST Studio Suite. A Time Domain Solver was used for the full-wave numerical calculations. To simulate an infinitely periodic array, we applied Periodic boundary conditions in the X and Y directions, while the Z direction (the direction of wave propagation) was set to an Open (add space) boundary. The structure was excited by a normally incident plane wave propagating along the negative Z-axis, with its electric field polarized along the Y-axis. To record the spectral response, we placed an E-Field Probe in the transmission path behind the structure and recorded the spectral plot of its Y-component electric field magnitude over a frequency range of 0.4 to 1.0 THz. By parametrically scanning the key geometric parameters of the structure (see Figure 1(a)), we ultimately obtained the dataset of corresponding spectral responses and structural parameters.

The performance of an inverse design model is highly dependent on the quality and coverage of the dataset. We selected the six geometric parameters that most significantly influence the EIT spectrum as variables. Within their physically feasible ranges, we employed a parameter sweep method to generate 1728 unique parameter combinations and performed batch simulations. To facilitate processing by the neural networks, each continuous spectrum was discretized at a fixed frequency interval into a 1202-point one-dimensional vector. Ultimately, we constructed a dataset of 1728 samples, where each sample consists of a 1202-dimensional spectral vector (the model input) and its corresponding 6-dimensional geometric parameter vector. Prior to being fed into the network, all spectral data and geometric parameters underwent Min-Max normalization to enhance the efficiency and stability of model training.

To achieve the inverse prediction from spectrum to parameters, we built and compared three deep learning models with distinct characteristics. The first, serving as a baseline, is a MLP, which learns the non-linear relationship between input and output by stacking multiple fully connected layers. The second is a 1D-CNN, which leverages convolutional kernels to automatically extract local features from the spectral data (such as the position, shape, and width of resonance peaks), giving it a natural advantage in processing sequential data. The third is a fully connected network incorporating residual connections (FC-ResNet). This architecture mitigates the vanishing gradient problem in deep network training via "shortcut connections," giving it the potential to learn deeper and more complex mappings between the spectra and parameters.

All models were trained and evaluated using the PyTorch framework. We randomly partitioned the dataset into training and test sets using a 50:50 ratio. The Mean Squared Error (MSE) was employed as the loss function, and the Adam optimizer was used for gradient descent and weight updates. During training, the model's performance was monitored on the test set after each epoch, and an Early Stopping strategy was implemented to prevent overfitting; specifically, training was terminated when the loss on the test set failed to improve for several consecutive epochs. Finally, the generalization ability and predictive accuracy of the trained models were objectively and impartially assessed on the independent test set using MSE and the coefficient of determination(R^2) as the final evaluation metrics.

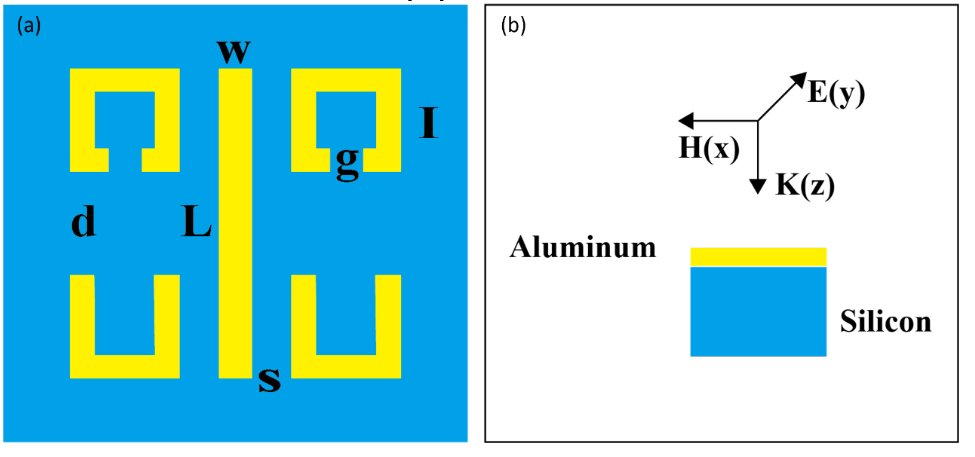

Figure 1. (a) Schematic of the THz EIT metamaterial unit cell, illustrating the key geometric parameters. (b) Side view of the structure, showing the Aluminum pattern on a Silicon substrate, along with the orientation of the incident electromagnetic field.

3. Results and Discussion

This section aims to provide a comprehensive presentation and analysis of the performance of the three proposed deep learning models on the THz EIT metamaterial inverse design task. We begin by quantitatively evaluating the overall predictive accuracy of the models using MSE and R^2. Subsequently, we intuitively demonstrate the physical validity of the models' predictions by performing forward simulations with the predicted geometric parameters. Finally, by analyzing the loss curves from the training process, we conduct an in-depth investigation into the learning behaviors and generalization capabilities of the different model architectures in a small-dataset environment, thereby elucidating the key rationale for model selection.

3.1. Quantitative Evaluation of Model Prediction Performance

To conduct an objective and standardized comparison of the predictive performance of the three models, we evaluated them on an independent test set. We employed MSE and R^2 as our core evaluation metrics. The MSE provides a direct measure of the average error between the predicted and true values, while the R^2 quantifies the model's ability to explain the variance in the data. Table 1 details the overall performance metrics obtained for the three models on the test set.

Table 1. Comparison of the predictive performance metrics for the three models (FC-ResNet, MLP, and 1D-CNN) on the independent test set.

Model	Train_MSE	Test_MSE	R^2
FC-ResNet	0.011617	0.020856	0.9794
MPL	0.027616	0.070423	0.9438
1D-CNN	0.030733	0.139951	0.8890

The quantitative results presented in Table 1 clearly indicate significant performance disparities among the three models. The FC-ResNet model demonstrated overwhelmingly superior performance across all evaluation metrics. Its Mean Squared Error on the test set (Test_MSE) was 0.020856, the lowest of all models, while its R^2 value reached as high as 0.9794. This indicates that the inverse model established by the FC-ResNet can explain nearly 98% of the variance in the dataset, achieving extremely high predictive accuracy. This exceptional performance can be attributed to its deep architecture and residual learning mechanism. We infer that for the EIT inverse problem investigated in this study, the overall morphology and global correlation features of the spectrum may be more critical than purely localized resonance peak characteristics. By constructing an "information highway," the FC-ResNet enables the effective training of a very deep fully connected network, thereby successfully capturing this complex, non-local mapping relationship that depends on global information.

The baseline MLP model's performance was intermediate, with an R^2 value of 0.9438. Although it is also capable of processing global information, its ability to learn complex mappings is inferior to that of the FC-ResNet due to the absence of residual connections, which leads to challenges such as vanishing gradients when training deep networks.

Contrary to theoretical expectations, the 1D-CNN model performed the worst in this experiment, with an R^2 value of only 0.8890. Although 1D-CNNs are adept at extracting local features from spectra using convolutional kernels, this result suggests that their architecture may also pose a risk of information loss. During the process of multi-layer convolution, and particularly through pooling operations, the model may discard subtle but crucial global information distributed across the entire spectrum in its effort to refine and compress features. Consequently, its specialization in local features became a limitation, leading to its subpar performance on this task, which requires a global perspective

3.2. Physical Validation and Visualization of Inverse Design Results

To intuitively validate the effectiveness of the model predictions from a physical standpoint, we moved beyond abstract statistical metrics and conducted a comparative analysis of reconstructed spectra. The core of this method involves randomly selecting a sample from the independent test set and using its "target spectrum" as input to predict the corresponding geometric parameters with each of the three trained models. Subsequently, these three sets of predicted parameters were used to perform forward electromagnetic simulations in CST Studio Suite, yielding three reconstructed spectra, which were then compared against the original target spectrum.

As can be clearly observed in Figure 2, the reconstructed spectrum generated from the parameters predicted by the FC-ResNet aligns almost perfectly with the target spectrum. An extremely high degree of consistency is maintained in the frequency positions and depths of the two absorption dips, as well as in the peak magnitude and overall lineshape of the central transparency window. This provides strong evidence that the prediction results from the FC-ResNet are physically accurate and reliable, demonstrating that it successfully learned the complex mapping relationship between the spectrum and the structure.

The reconstructed spectrum from the baseline MLP model generally matches the overall trend of the target spectrum but exhibits noticeable deviations in detail. For instance, there is a slight frequency shift in its predicted resonance frequencies (the positions of the absorption dips), and the peak magnitude matching is inferior to that of the FC-ResNet. This is consistent with its intermediate performance in the quantitative evaluation.

The 1D-CNN model performed the worst. There are significant discrepancies between its reconstructed spectrum and the target spectrum, with severe inaccuracies, particularly in the prediction of the resonance frequencies. This visually confirms that although 1D-CNNs are theoretically suitable for sequential data, for this specific task, the architecture may have inappropriately discarded global information crucial for accurate inversion, leading to physically unreliable prediction results.

In summary, the comparative results of the reconstructed spectra provide strong physical evidence to support our quantitative evaluation. It clearly demonstrates that the FC--ResNet not only leads in statistical metrics but, more importantly, is capable of generating design parameters that are physically valid and can accurately reproduce the target optical response, showcasing its immense potential for solving such complex inverse design problems.

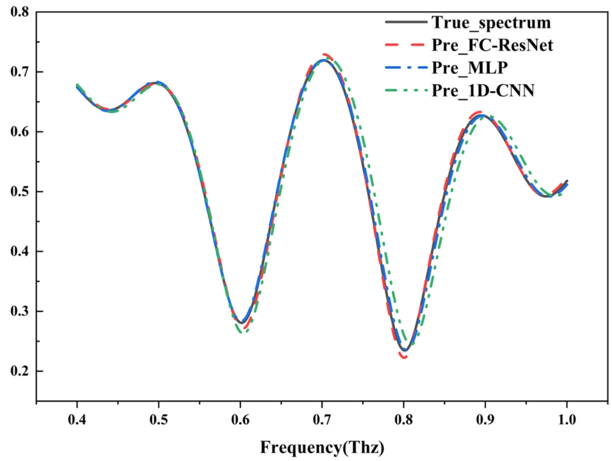

Figure 2. Comparison of the target spectrum (True_spectrum) with the reconstructed spectra generated from the parameters predicted by the three models (FC-ResNet, MLP, and 1D-CNN) for a representative test sample.

3.3. Discussion on Generalization Ability and Small-Dataset Challenges

One of the central challenges of this research was to train a model with good generalization ability on a small dataset consisting of only 1728 samples. Figure 3 displays the loss function curves for the three models during the training process, which provides a window into understanding their learning behaviors and generalization capabilities.

As shown in Figure 3, the training loss of the MLP drops rapidly to a very low level in the initial stages of training, but its test loss quickly plateaus, creating a significant "generalization gap" between the two curves. This is a classic example of overfitting: due to an excess of parameters and insufficient structural constraints, the model begins to "memorize" specific noise and coincidental features in the training data rather than learning the underlying physical principles, leading to poor performance on unseen test data. The situation improves with the FC--ResNet, which exhibits a smaller generalization gap than the MLP, although one is still present.

In stark contrast are the loss curves of the 1D-CNN. Its training and test losses remain closely synchronized throughout the entire training process, decreasing together and converging smoothly. This indicates that the 1D-CNN model possesses excellent generalization ability, having successfully learned a universal spectrum-to-structure mapping from the limited training samples. This is primarily attributed to two intrinsic properties of convolutional networks: local connectivity and weight sharing. Local connectivity allows each neuron to process only a small portion of the input, focusing on local features, while weight sharing means the same convolutional kernel (feature extractor) is reused across the entire spectrum, drastically reducing the total number of parameters the model needs to learn. This architectural "inductive bias" is highly compatible with the physical properties of spectral data, acting as a built-in and highly effective form of regularization that fundamentally suppresses the model's tendency to overfit on a small dataset. Therefore, our results strongly suggest that when faced with a data-sparse physical inverse design problem, selecting a parameter-efficient network architecture with the correct inductive bias is far more critical and effective than simply increasing the depth or complexity of a general-purpose model.

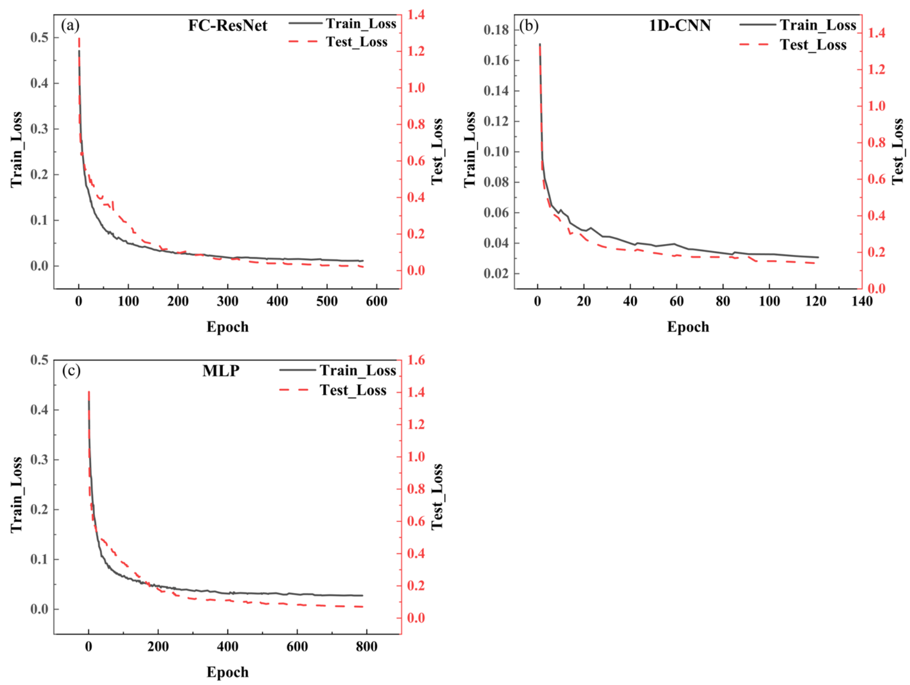

Figure 3. Training and test loss curves for the three models during the training process: (a) FC-ResNet, (b) 1D-CNN, and (c) MLP. The significant gap between the training loss and test loss for the MLP indicates overfitting

4. Conclusion

This paper addresses the challenges of inefficiency, high computational cost, and strong dependence on designer experience inherent in traditional design methods for THz EIT metamaterials. We proposed and validated an inverse design solution based on deep learning for small datasets. By constructing a spectrum-structure parameter dataset of 1728 samples using the CST Studio Suite electromagnetic simulation software, we systematically trained, evaluated, and compared three different neural network models: an MLP, an FC-ResNet, and a 1D-CNN.

The research findings clearly indicate that for this EIT metamaterial inverse design task, the FC-ResNet model exhibited the optimal predictive performance, achieving an R^2 value as high as 0.9794, which was significantly superior to both the MLP and the 1D-CNN. This discovery suggests that for such complex physical problems, the inverse mapping relationship may depend more on the global, holistic features of the spectrum rather than solely on localized resonance peak information. The

FC-ResNet, by virtue of its deep architecture and effective residual learning mechanism, successfully captured this high-dimensional, non-linear mapping.

The core contribution of this study lies in its empirical demonstration that when selecting a model for a physical inverse design problem, one cannot rely solely on theoretical architectural suitability but must also consider the complexity of the actual problem. The results emphasize that a deep model with sufficient expressive power that can be trained stably may hold an advantage in handling complex mappings dependent on global information, compared to a more specialized architecture that risks information loss. This provides a crucial practical guide for selecting and optimizing inverse design models under resource-constrained conditions, offering an efficient and feasible solution to accelerate the development of novel THz functional devices.

Despite the positive outcomes of this study, certain limitations remain that offer avenues for future work. First, the current dataset is based entirely on ideal electromagnetic simulations and does not account for potential fabrication errors that may occur in practice. Future research could incorporate manufacturing tolerances as random variables into the dataset to train more robust models. Second, more advanced network architectures could be explored, such as generative models like Generative Adversarial Networks (GANs) or Variational Autoencoders (VAEs), which could not only predict parameters but also directly generate novel, high-performance structural topologies based on performance requirements. Finally, the methodology validated in this research possesses good universality and can be extended in the future to other types of metamaterials (such as absorbers and chiral structures) and even to a broader range of inverse design problems in photonics and physics.

References

[1] Tonouchi, Masayoshi. "Cutting-edge terahertz technology." Nature photonics 1.2 (2007): 97-105.

[2] Ferguson, Bradley, and **-Cheng Zhang. "Materials for terahertz science and technology." Nature materials 1.1 (2002): 26-33.

[3] Chen, Hou-Tong, Antoinette J. Taylor, and Nanfang Yu. "A review of metasurfaces: physics and applications." Reports on progress in physics 79.7 (2016): 076401.

[4] Smith, David R., John B. Pendry, and Mike CK Wiltshire. "Metamaterials and negative refractive index." science 305.5685 (2004): 788-792.

[5] Zhang, Shuang, et al. "Plasmon-induced transparency in metamaterials." Physical review letters 101.4 (2008): 047401.

[6] Chiam, Sher-Yi, et al. "Analogue of electromagnetically induced transparency in a terahertz metamaterial." Physical Review B—Condensed Matter and Materials Physics 80.15 (2009): 153103.

[7] Singh, Ranjan, et al. "Coupling between a dark and a bright eigenmode in a terahertz metamaterial." Physical Review B—Condensed Matter and Materials Physics 79.8 (2009): 085111.

[8] Liu, Na, et al. "Planar metamaterial analogue of electromagnetically induced transparency for plasmonic sensing." Nano letters 10.4 (2010): 1103-1107.

[9] Molesky, Sean, et al. "Inverse design in nanophotonics." Nature Photonics 12.11 (2018): 659-670.

[10] Ma, Wei, et al. "Deep learning for the design of photonic structures." Nature photonics 15.2 (2021): 77-90.

[11] Peurifoy, John, et al. "Nanophotonic particle simulation and inverse design using artificial neural networks." Science advances 4.6 (2018): eaar4206.

[12] Liu, D., Tan, Y., Khoram, E., & Yu, Z. Training deep neural networks for the inverse design of nanophotonic structures. Acs Photonics, 5(4), 1365-1369.

[13] Nadell, Christian C., et al. "Deep learning for accelerated all-dielectric metasurface design." Optics express 27.20 (2019): 27523-27535.

[14] Jiang, Jiaqi, et al. "Free-form diffractive metagrating design based on generative adversarial networks." ACS nano 13.8 (2019): 8872-8878.

[15] Pestourie, Raphaël, et al. "Active learning of deep surrogates for PDEs: application to metasurface design." npj Computational Materials 6.1 (2020): 164.

[16] Liu, Zhaocheng, et al. "Generative model for the inverse design of metasurfaces." Nano letters 18.10 (2018): 6570-6576.

[17] Ma, Wei, et al. "Probabilistic representation and inverse design of metamaterials based on a deep generative model with semi - supervised learning strategy." Advanced Materials 31.35 (2019): 1901111.

[18] Asano, Takashi, and Susumu Noda. "Optimization of photonic crystal nanocavities based on deep learning." Optics express 26.25 (2018): 32704-32717.

[19] LeCun, Yann, et al. "Gradient-based learning applied to document recognition." Proceedings of the IEEE 86.11 (2002): 2278-2324.

[20] He, Kaiming, et al. "Deep residual learning for image recognition." Proceedings of the IEEE conference on computer vision and pattern recognition. 2016.