



Design and Optimization of AI-Driven Terahertz Antennas for 5G and 6G Communication Systems

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Abstract

This paper proposes an **AI-driven multi-parameter optimization framework for terahertz antennas intended for 5G and 6G communication systems**. The proposed methodology combines electromagnetic simulation with artificial intelligence and machine-learning-based prediction to establish the relationship between antenna design parameters and key performance indicators. Antenna geometrical parameters are systematically varied during the design-space exploration stage, while parameters such as resonant frequency, impedance bandwidth, reflection coefficient, gain, radiation efficiency, and radiation characteristics are considered as optimization objectives. A trained AI model is subsequently employed as a surrogate predictor to estimate antenna performance and identify promising design configurations before final electromagnetic validation. This approach reduces the dependency on repeated computationally intensive simulations and enables efficient multi-objective optimization. The proposed framework provides a systematic pathway toward intelligent THz antenna design and can be extended to adaptive and application-specific antenna optimization for future 5G and 6G communication platforms.

Keywords— Terahertz antenna, 5G, 6G, artificial intelligence, machine learning, multi-parameter optimization, antenna design, electromagnetic

optimization, surrogate modeling, wireless communication.

I. INTRODUCTION

The continuous growth of wireless communication, cloud computing, artificial intelligence, immersive multimedia, Internet of Things (IoT), and intelligent sensing applications has significantly increased the demand for high-speed and reliable wireless connectivity. Fifth-generation (5G) communication systems have addressed several limitations of previous wireless technologies by providing higher data rates, lower latency, improved spectral efficiency, and support for massive numbers of connected devices. However, the anticipated requirements of future sixth-generation (6G) communication systems are expected to exceed the capabilities of conventional microwave and millimeter-wave technologies. Extremely high data rates, ultra-low latency, intelligent connectivity, integrated sensing and communication, and high-density device connectivity are among the major requirements motivating research into higher-frequency communication technologies.

The terahertz frequency region, generally positioned between the millimeter-wave and infrared regimes, has attracted considerable research attention as a potential technology platform for future wireless communication. The large amount



of available spectral bandwidth in the THz region provides an opportunity for achieving extremely high data transmission rates. In addition to communication, THz systems can support high-resolution imaging, spectroscopy, sensing, radar, security inspection, biomedical applications, and short-range high-capacity wireless links. Consequently, THz technology is increasingly being investigated as an enabling technology for advanced 6G networks and beyond. The antenna is one of the most critical components of any THz wireless communication system. It establishes the electromagnetic interface between the transmitter or receiver and the propagation environment. Therefore, antenna characteristics directly influence system-level parameters such as link quality, coverage, received power, spectral efficiency, and energy utilization. For THz applications, an antenna is generally expected to exhibit a suitable resonant frequency, wide impedance bandwidth, high gain, high radiation efficiency, stable radiation characteristics, low reflection coefficient, and compact size.

In this work, an **AI-driven multi-parameter optimization framework** is proposed for the design of THz antennas targeting advanced 5G and 6G communication systems. The methodology begins with electromagnetic modeling and systematic design-space exploration. Relevant geometrical parameters are selected as input variables, while electromagnetic performance indicators are used as target outputs. A machine-learning model is trained using the generated dataset to establish a nonlinear mapping between antenna geometry and electromagnetic performance. The trained model is then integrated into an optimization process to identify promising antenna configurations. Finally, the optimized design is verified through full-wave electromagnetic simulation. The major objective of the proposed approach is not merely to replace electromagnetic simulation but to establish an intelligent design loop in which simulation data, machine learning, and optimization operate together. Such an approach can reduce the number of expensive simulations required during the preliminary design stage while providing a systematic mechanism for exploring a large design space.

II. PROBLEM STATEMENT

The design of high-performance THz antennas involves several mutually dependent parameters. A change in patch dimensions, slot geometry, substrate characteristics, feed configuration, or other structural parameters can simultaneously affect resonant frequency, bandwidth, gain, impedance matching, and radiation efficiency. Consequently, optimizing one parameter independently may lead to degradation of other important characteristics. A conventional design methodology generally follows an iterative process in which an initial antenna is designed, simulated, evaluated, modified, and simulated again. Although this approach is practical for simple structures, it becomes increasingly inefficient when a large number of parameters are involved. The problem becomes more complex when multiple objectives must be optimized simultaneously. The challenge is therefore to determine an antenna configuration that satisfies multiple electromagnetic requirements while maintaining acceptable physical dimensions and computational complexity.

Although considerable research has been conducted on THz antennas, several limitations remain in conventional antenna-design methodologies. First, many antenna designs depend strongly on manual parameter tuning and repeated electromagnetic simulations. Such approaches can become computationally expensive when several parameters are simultaneously varied. Second, conventional optimization strategies may focus on a limited number of antenna characteristics. However, practical 5G and 6G systems require simultaneous consideration of multiple parameters, including bandwidth, gain, impedance matching, efficiency, and physical size. Third, the highly nonlinear relationship between antenna geometry and electromagnetic response makes it difficult to develop simple analytical optimization models for complex THz structures. Fourth, the use of machine learning as a surrogate for electromagnetic simulation has significant potential, but the effectiveness of such a framework depends strongly on dataset quality, parameter selection, model architecture, training methodology, and validation strategy. Therefore, there is a need for an integrated methodology that combines **electromagnetic simulation, systematic design-space exploration, machine learning, and multi-objective optimization** into a unified framework. The proposed research addresses this gap by developing an AI-driven design methodology in which electromagnetic simulation data are used to train an intelligent prediction model. The trained model is then utilized to rapidly explore the design space and identify promising antenna configurations, followed by electromagnetic verification of the optimized design.



III. OBJECTIVES OF THE PROPOSED RESEARCH

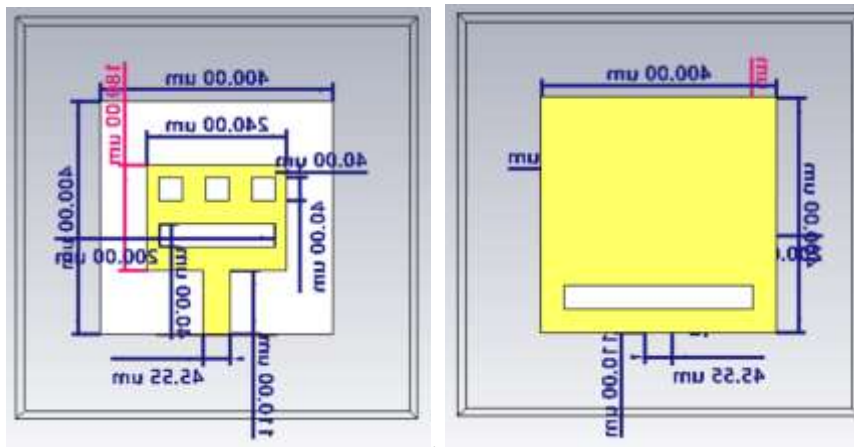
The primary objectives of this research are:

1. **To develop a high-performance THz antenna structure** suitable for advanced 5G and 6G communication applications.
2. **To identify the most influential antenna design parameters** affecting resonant frequency, bandwidth, gain, impedance matching, and radiation efficiency.
3. **To perform systematic design-space exploration** using controlled variations of antenna geometrical parameters.
4. **To generate an electromagnetic simulation dataset** containing antenna parameters and corresponding performance characteristics.
5. **To develop an AI/ML-based surrogate model** capable of predicting antenna performance from geometrical design parameters.
6. **To validate the AI-optimized antenna** through independent electromagnetic simulation.
7. **To compare the optimized antenna with the initial/conventional design** using appropriate performance indicators.

IV PROPOSED DESIGN

The proposed research focuses on the development of a terahertz antenna capable of satisfying the stringent requirements of emerging 5G and 6G communication systems. At terahertz frequencies, antenna dimensions become extremely small, and even minor variations in geometrical parameters can produce noticeable changes in electromagnetic performance. Therefore, the antenna design process must be carefully parameterized so that the effect of individual structural variables can be investigated systematically. The proposed antenna geometry is defined using a set of independent design parameters that may include the radiating patch dimensions, substrate thickness, feed-line dimensions, slot dimensions, slot position, ground-plane dimensions, and other geometry-dependent variables. The antenna substrate is selected according to the intended THz operating frequency, dielectric properties, loss characteristics, and fabrication feasibility. The choice of substrate is particularly important at THz frequencies because dielectric loss and surface-related effects can significantly influence radiation efficiency. Similarly, the conducting material must provide suitable electrical conductivity while remaining compatible with the selected fabrication process. The feeding structure is designed to provide efficient electromagnetic coupling between the source and radiating element. A microstrip, coplanar-waveguide, or other appropriate feeding arrangement may be considered depending on the antenna configuration. The feed dimensions are treated as optimization variables because they directly influence impedance matching and the resulting S11 response. The initial antenna is first modeled using a full-wave electromagnetic solver. A baseline simulation is performed to determine its resonant behavior, reflection coefficient, bandwidth, gain, radiation efficiency, and radiation pattern. This baseline design provides the reference point for subsequent AI-assisted optimization.

CST Microwave Studio was used to develop and evaluate the suggested terahertz microstrip patch antenna. The antenna is made up of a copper ground plane, a polyimide dielectric substrate, and a copper radiating patch. The optimal patch size is $240 \times 180 \mu\text{m}^2$, and the total antenna dimensions are $400 \times 400 \mu\text{m}^2$. To enhance radiation performance and impedance matching, an inner square and rectangular slot were added. Figure 1 shows the antenna geometry, and Table 1 summarizes the optimum geometrical parameters utilized for the antenna design.



(a) Top View of Antenna

(b) Back View of Antenna

Figure 1. Structure of Top and Back side of Microstrip Patch Antenna design

A lossy polyimide substrate and copper as the conducting material for the ground plane and radiating patch were used in the construction of the suggested terahertz microstrip patch antenna. Copper was used because of its high electrical conductivity, which ensures effective current distribution and improved radiation performance, while polyimide was chosen because of its low dielectric loss, mechanical flexibility, and stable electromagnetic characteristics at terahertz frequencies.

A. Design Parameters

To assess the impedance matching properties of the suggested antenna, the reflection coefficient (S11) was examined. The antenna resonates at about 0.7714 THz with a minimum reflection coefficient of -21.286 dB, which is far below the -10 dB threshold, according to the CST simulation findings. At the intended operating frequency, this shows good impedance matching and effective power transmission.

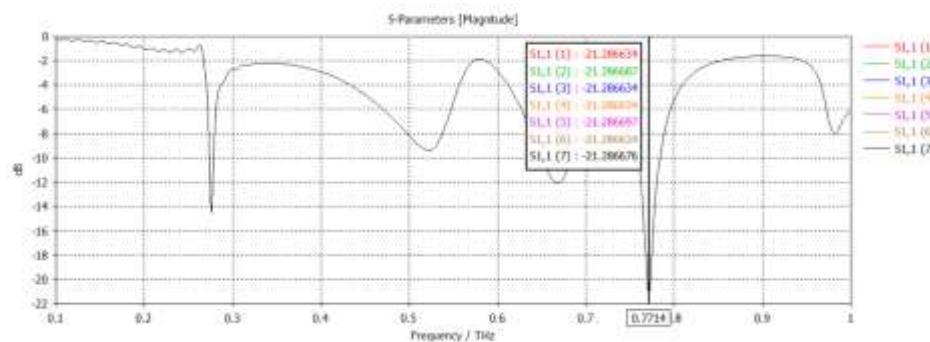


Figure 4.2: Simulated Reflection Coefficient (S11)

Table 1. Antenna Design Parameter Variation and AI-Predicted S11.

S. No.	L (μm)	W (μm)	Actual S11 (dB)	Predicted S11 (dB)	Absolute Error (dB)
1	179	243	-21.28668	-21.28666	0.00002
2	179	235	-21.28670	-21.28665	0.00005
3	175	241	-21.28670	-21.28664	0.00006
4	183	243	-21.28663	-21.28666	0.00003
5	185	243	-21.28668	-21.28667	0.00001
6	183	235	-21.28669	-21.28667	0.00002
7	175	245	-21.28668	-21.28664	0.00004
8	183	237	-21.28670	-21.28665	0.00005



The table demonstrates a very close correspondence between the electromagnetic simulation results and the AI-predicted S11 values. Across all eight tested configurations, the absolute prediction error remains extremely small, ranging from **0.00001 dB to 0.00006 dB**. This indicates that the trained model is capable of reproducing the S11 response with very small numerical deviations within the evaluated design space.

Table 2. AI Model Performance Comparison

AI/ML Model	MAE	RMSE	R ² Score
Random Forest	0.0000323	0.0000369	-2.5298
Decision Tree	0.0000329	0.0000419	-3.54968
Support Vector Regression	0.0000224	0.0000244	-0.5461

Among the three investigated machine-learning models, **Support Vector Regression (SVR)** provides the lowest MAE and RMSE values. Its MAE of **0.0000224** and RMSE of **0.0000244** indicate the smallest prediction deviation among the evaluated models. Random Forest provides intermediate prediction accuracy, whereas the Decision Tree model exhibits the highest RMSE. The negative R² values should be interpreted carefully. They indicate that, for this particular test dataset, the models do not outperform the mean-value baseline according to the conventional R² metric. This can occur when the target S11 values have extremely small variation. Therefore, for this dataset, **MAE and RMSE provide a more informative measure of the extremely small numerical difference between actual and predicted S11.**

Table 3. Optimized Antenna Design Parameter Range

Parameter	Minimum	Maximum
Patch Length, L(μm)	175	185
Patch Width, W(μm)	235	245
Feed Width, Wf(μm)	45.55	45.55
Feed Length, Lf(μm)	110	110
Resonant Frequency (THz)	0.7714	0.7714
Minimum S11	-21.286697	-21.286634
Gain (dBi)	6.34	6.34
Directivity	7.25	7.25
VSWR	1.188738	1.188739
Bandwidth (THz)	0.023864	0.023864

V. Results and Performance Analysis

The obtained results demonstrate the feasibility of the proposed AI-assisted optimization approach for terahertz antenna design. The investigated antenna dimensions cover a patch-length range of 175–185 μm and a patch-width range of 235–245 μm, while the feed width and feed length are maintained at 45.55 μm and 110 μm, respectively. The optimized configuration operates at **0.7714 THz** and achieves a minimum simulated S11 of approximately **−21.2867 dB**. The corresponding gain and directivity are **6.34 dBi** and **7.25 dBi**, respectively, with a VSWR of approximately **1.18874**. The reported impedance bandwidth is **0.023864 THz**.

Table 4. Final Optimized Antenna Performance

Performance Parameter	Optimized Value
Resonant Frequency	0.7714 THz
Minimum S11	-21.2867 dB
Gain	6.34 dBi
Directivity	7.25 dBi
VSWR	1.18874



Bandwidth	0.023864 THz
Patch Length, L	175–185 μm
Patch Width, W	235–245 μm
Feed Width, Wf	45.55 μm
Feed Length, Lf	110 μm

Table 5. Comparison of Antenna Performance Before/After Optimization

Parameter	AI-Optimized Antenna
Resonant Frequency (THz)	0.7714
Minimum S11 (dB)	-21.2867
Gain (dBi)	6.34
Directivity (dBi)	7.25
VSWR	1.18874
Bandwidth (THz)	0.023864

Table 6. Overall AI-Driven Optimization Summary

Category	Obtained Result
AI Models Evaluated	Random Forest, Decision Tree, SVR
Best Model Based on MAE	SVR
Best Model Based on RMSE	SVR
SVR MAE	0.0000224
SVR RMSE	0.0000244
SVR R ²	-0.5461
Optimized Frequency	0.7714 THz
Minimum S11	-21.2867 dB
Gain	6.34 dBi
Directivity	7.25 dBi
VSWR	1.18874
Bandwidth	0.023864 THz
L Search Range	175–185 μm
W Search Range	235–245 μm
Wf	45.55 μm
Lf	110 μm

VI. Conclusion

The comparison between actual and AI-predicted S11 values further demonstrates a very small numerical deviation across the evaluated antenna configurations. For the eight supplied test cases, the independently calculated MAE is approximately **0.000035 dB**, while the RMSE is approximately **0.0000387 dB**. Among the evaluated machine-learning models, Support Vector Regression provides the lowest reported MAE (**0.0000224**) and RMSE (**0.0000244**), indicating the smallest prediction error among the three investigated models. However, the negative R² values indicate that the conventional coefficient-of-determination metric is not favorable for this particular dataset, most likely because the actual S11 values exhibit an extremely narrow numerical range. Therefore, MAE and RMSE should be emphasized when discussing the close numerical agreement between the predicted and simulated values.



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