

Design And Optimization Of AI Based Massive MIMO Antenna System For Next Generation Communication System

¹Dr. N B Gohil*, ²Prof. Rushi J. Trivedi, ³Dr. Dhara J. Sangani, ⁴Dr. Devang G. Jani,
⁵Dr. Dhaval R. Bhojani

¹Associate Professor, Government Engineering College, Rajkot, Gujarat-360005, India

²Assistant Professor, Government Engineering College, Rajkot, Gujarat-360005, India

³Assistant Professor, Vishwakrama Government Engineering College, Chandkheda, Gujarat

⁴Associate Professor, ⁴Government Engineering College, Bhavnagar, Gujarat

⁵Assistant Professor ⁵Government Engineering College, Rajkot, Gujarat

*Corresponding Author: Dr. N B Gohil

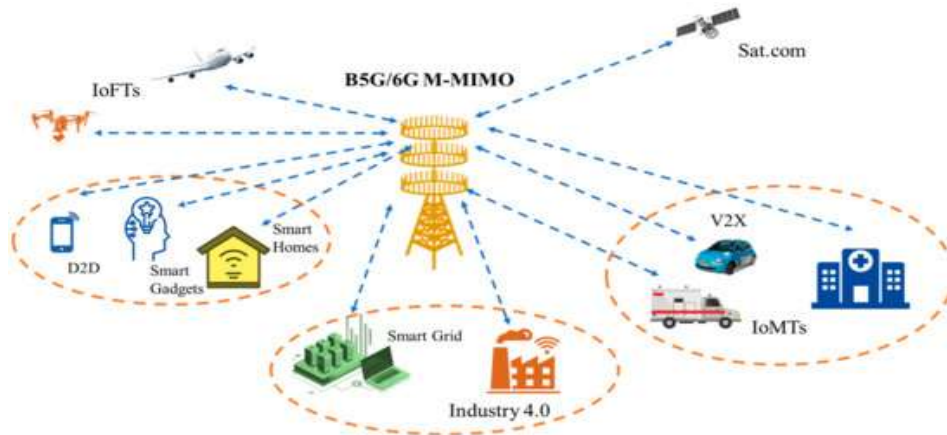
Abstract

The rapid advancement of wireless communication has intensified the demand for high data rates, low latency, and energy-efficient systems, driving research into Massive MIMO (M-MIMO) antennas for 5G and 6G. However, challenges such as interference, poor isolation, and hardware complexity persist. To address these, this work integrates Artificial Intelligence (AI) with graphene-based M-MIMO antenna design, enabling optimization through data-driven models. The methodology begins with single-element graphene-copper patch structures on a polyamide substrate, progressively optimized to a two-port MIMO configuration. Repeated simulations generate datasets for training regression-based machine learning models, including Decision Tree, Random Forest, XGBoost, Lasso, and Poisson regressions. Parametric analysis was conducted using CST simulations, systematically varying substrate thickness, length, and patch dimensions. The proposed design achieved a maximum gain of 16 dB at 9 THz, deep reflection coefficient (S_{11}) of -65 dB, isolation (S_{21}) between -20 and -60 dB, ECC below 0.03, and diversity gain (DG) around 10 dB. Channel capacity loss (CCL) remained under 0.2 bits/s/Hz, and TARC stayed below -20 dB. Among ML models, XGB Regression outperformed others, with MAE of 3.10%, RMSE of 3.25%, and R^2 of 98.20%, confirming reliable performance prediction and efficient design optimization.

Keywords: MIMO, Artificial Intelligence, CCL, Machine Learning, ECC, TARC

1. Introduction

The rapid evolution of Wireless Communication Systems (WCS) has produced an ever-increasing demand for high data rates, increased spectral efficiency, low latency, and dependable connectivity, which are the fundamental needs of future communication systems like 5G and beyond [1,2]. "Massive Multiple-Input Multiple-Output (M-MIMO)" technology is one such disruptive innovation that addresses these challenges by developing a huge number of antenna elements at the base station to support multiple users at the same time using the same frequency band [3]. Through spatial multiplexing and beamforming features, M-MIMO greatly enhances spectrum use, energy efficiency, and system throughput [4]. However, the behavior of M-MIMO systems is intrinsically subject to the antenna array's design and optimization, which directly impacts parameters like gain, radiation pattern, directivity, mutual coupling, and overall system efficiency [5,6]. The M-MIMO in B5G/6G heterogeneous networks is shown in Figure 1.

Figure 1: Utilising M-MIMO in heterogeneous networks for B5G/6G[7].

The Artificial Intelligence (AI) approaches for antenna design and optimization have further disrupted the field by allowing adaptive, data-driven, and cognitive decision-making to tackle complex electromagnetic problems [8,9]. AI algorithms, and more specifically algorithms related with “Machine Learning (ML)” and “Deep Learning (DL)”, have been shown to be optimal in terms of temporal efficiency with respect to optimizing antenna parameters, predicting performance, and working around nonlinear design problems that cannot be effectively tackled with established methods [10]. In addition, AI-driven optimization leads to less design time, lower computational and experimental costs, along with more robust and repeatable performance of antennas throughout a range of propagation environments [11,12].

In next-generation communication systems, the combination of AI and M-MIMO antenna technology could help solve problems related to interference mitigation, energy use, hardware complexity, and channel estimation accuracy [13]. AI's ability to learn from real-time data and dynamically reconfigure antenna arrays allows for the flexibility to adapt to varying traffic demands, mobility patterns, and spectrum availability, thus providing the flexibility needed for communication infrastructure of the future. The design and optimization of AI-based M-MIMO antenna systems represent a great opportunity to increase coverage, capacity, and user experience in future wireless networks [14,15].

The development of effective antennas for MIMO systems is critical to the progress of high-frequency communication systems, where the most important parameters such as “bandwidth, gain, isolation, efficiency, and ECC” need to be enhanced. The new volume of literature depicts tremendous progress in MIMO antenna design for 5G, 6G, and THz communication systems with great emphasis on compact size, high gain, and ML optimization. Patel et al. (2025) [16] designed a unique Double Graphene Stripline Slot Patch (DGSSP-MIMO) antenna with working frequencies at 4.71, 8.55, and 9 THz, in which the inclusion of graphene enhanced confinement with S_{11} of -37.28 dB but at the expense of compromised gain, whereas ML tuning provided $R^2 = 0.9768$. Likewise, Haque et al. (2025) [17] introduced a THz-band MIMO antenna for IoT with high efficiency ($>96.5\%$), great isolation (>-44 dB), and miniaturized size, for which Gradient Boosting Regression offered $>98\%$ prediction accuracy in isolation. Ananta et al. (2025) [18] proposed a dual-band mm-wave MIMO antenna (28/38 GHz) which transitioned to a 4-port design with high bandwidth, isolation >29 dB, and $>99\%$ radiation efficiency, Extra Trees Regression predicting the isolation with $\sim 93\%$ accuracy.

Additionally, Haque et al. (2025) [19] and Haque et al. (2024) [20] optimized 28–38 GHz mm-wave microstrip patch MIMO antennas by using supervised regression and Gaussian Process Regression (GPR), with high gains (>10 dB), broad bandwidths, and ML-based performance predictions. Kumar et al. (2023) [21] and Ud Din et al. (2023) [22] suggested miniature THz and mm-wave MIMO structures utilizing defected ground and frequency-selective surfaces (FSS), with up to 30 dB isolation improvement and increased gain (>8.6 dBi). Dwivedi et al. (2023) [23] further developed this with LHCP/RHCP dual-port sub-6 GHz MIMO antenna utilizing ML-optimized DGS with $R^2 = 0.82$ and $ECC < 0.005$, achieving successful polarization diversity.

At higher frequency ranges, substantial innovations focus on compactness, broad bandwidth, and sophisticated ML integration. Amraoui et al. (2024) [24] developed an 128/178 GHz dual-frequency MIMO array based on DGS with compact size, $ECC < 0.012$, and diversity gain close to 10 dB. Al-Bawri et al. (2025) [25] introduced an eight-port wideband THz-MIMO antenna with $ECC < 0.01$, $DG > 9.99$ dB, $TARC < -10$ dB, and ridge regression-based predicted gain with ~98% accuracy. Their follow-up work (2024) [26] presented a compact polyimide-based 6G THz antenna with high gain (15 dB), isolation >31 dB, efficiency >97%, and RFR achieving >95% accuracy in gain prediction. Asaad et al. (2024) [27] used graphene-based hexagon ring MIMO antennas for 6G, using DGS and NL decoupling to achieve isolation of 23 dB, $ECC \sim 0.0048$, and efficiency of 98%. Combined, these works emphasize the importance of graphene integration, defected ground structure, compact geometries, and ML-based optimization towards obtaining high-performance MIMO antenna systems. Table 1 present the performance comparison of previous work.

Table 1: Comparison of performance with corresponding works

Auth ors (Yea r)	Reson ance	Band width	Isola tion	Gain	Effici ency	ECC	DG	Substr ate Materi al	ML Applied
Patel et al. (202 5)	4.71, 8.55, 9 THz	Multib and	– 37.27 dB (S11)	12.94 dB (w/o graph ene), 8.46 dB (with graph ene)	<70%	0.003	10	Graph enestri pline slot patch	Yes (ML optimiz ation, $R^2=0.97$)
Haqu e et al. (202 5)	6.51, 7.48, 8.46 THz	0.7, 0.69, 0.89 THz	>32 dB, >44 dB, >45 dB	13.53 dBi	>96.5 %	NA	9.9 9 dB	Polyim ide substr ate (160× 75 μm^2)	Yes (Gradi ent Boostin g, >98% acc.)
Anan ta et al. (202	28 & 38 GHz	2.55 GHz, 5.77 GHz	>35 dB, >29 dB	9 dB, 8.4 dB	98– 99%	0.001	–	Rogers RT588 0	Yes (Extra Trees, ~93%

5)									acc.)
Haque et al. (2025)	28–32.2 & 36.5–40.7 GHz	Wideband	>29 dB	10.14 dBi	95%	NA	9.99 dB	Rogers RT5880	Yes (Random Forest)
Kumar et al. (2023)	2.2 THz	1.74–2.52 THz	30 dB max	4.4	92%	0.006	9.998 dB	Polyimide	No
Uddin et al. (2023)	28 GHz	1.6 GHz	>26 dB	7.2 dBi (w/o FSS), 8.6 dBi (w/ FSS)	NA	<0.002	>9.99 dB	Rogers RT/Duroid	No
Dwivedi et al. (2023)	3.0–4.2 GHz	1.2 GHz (IBW)	25	4	95%	<0.005	~9.99 dB	Rogers substrate	Yes (ANN, $R^2=0.82$)
Haque et al. (2024)	28 GHz	4.64	>26 dB	10.34 dBi	98.35	0.0005	9.99 dB	Rogers RT5880	Yes (GPR, best acc.)
Amraoui et al. (2024)	128 & 178 GHz	0.00598, 0.00613 THz	–25	5.16 & 6.24 dB	90%	<0.012	~10 dB	Polyimide	No
Al-Bawri et al. (2025)	0.9–1.68 THz	0.78	–10 dB TARC, CCL<0.2	>7.5 dBi	98%	<0.01	>9.99 dB	Polyimide (130×110 μm^2)	Yes (Ridge Regression, 98% acc.)
Al-Bawri et al. (2024)	Sub-THz & THz bands	1	>31 dB	15 dB	97.4 %	<0.0012	>9.99 dB	Polyimide	Yes (RFR, >95% acc.)
Asaad et al. (202	2.8 THz band	NA	23 dB	NA	98%	0.004859	9.99 dB	Graphene	No

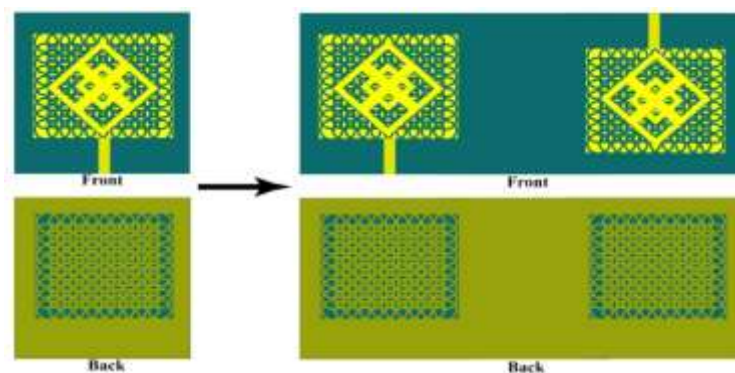
4)									
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The objective of this research is to exploit new AI-enabled methodologies in the optimization of M-MIMO antenna arrays, with the aim of improving their overall electromagnetic performance, optimizing resource allocation and scalability for large scale deployment, for future communication networks. The proposed research aims to address these challenges and leverage the combination of AI with M-MIMO technology, by contributing to the future development of WCS that are highly intelligent, energy efficient and can be relied on for future applications including autonomous systems, smart cities, immersive media, and the Internet of Things (IoT).

2. Design Methodology

Figure 2 shows the development of the design process from a single-element antenna (SEA) to a MIMO configuration, which is a significant step in the pursuit to improve antenna technology for upcoming 6G applications. This advancement is driven by their pursuit for improved performance, efficiency, and flexibility in WCS. Transforming from a SEA to MIMO allows us to use multiplexing advantages, spatial diversity, and enhanced spectrum efficiency, consequently addressing the rapidly increasing needs for elevated reduced latency, data rates, and expanded network capacity in 6G networks [28].

Figure 2: Procedures for creating an antenna (a) Single element; (b) MIMO Antenna



The careful selection of materials for the antenna components is fundamental to this progression. Graphene is used as the material for the patch due to its great conductivity, mechanical strength, and flexibility [29]. To further improve the antenna's electromagnetic characteristics and conductivity, copper is used as the grounding element. This allows for efficient radiation efficiency and signal grounding.

In addition, the substrate material is polyamide, which is selected for its good dielectric qualities, such as a low-loss tangent of 0.0029 and a dielectric constant of 4.3. The polyamide substrate provides the best possible signal transmission with the least amount of signal attenuation and energy loss with regard to its 23 millimeter thickness. The antenna design showcases a comprehensive strategy to attaining high-performance WCS that are customized for the requirements of future 6G applications by utilizing the different properties of this material.

2.1 Single-element antenna

The antenna design process starts with meticulous attention, starting with the development of a single element antenna. Figure 3 illustrates the suggested SEA. The initial phase involves meticulous evaluation of material choices, with graphene

identified as the optimal choice for the patch element. Graphene, with its high electrical conductivity and mechanical resilience, is placed on top of the substrate to ensure the antenna performs at its best. However, copper is purposefully placed on the other side of the substrate to act as the grounding element. Accurate measurements are crucial for achieving the best possible signal transmission and attenuation reduction, with a substrate thickness of 11μm and patch and ground elements of 2μm. To determine the size of the patch, researchers use the following equation [30]:

$$\lambda = \frac{c}{f}$$

$$\epsilon_{eff} = \left(\frac{\epsilon_r + 1}{2} + \frac{\epsilon_r - 1}{2} \right) \times \left(1 + 12 \times \frac{h}{W} \right)^{-0.5}$$

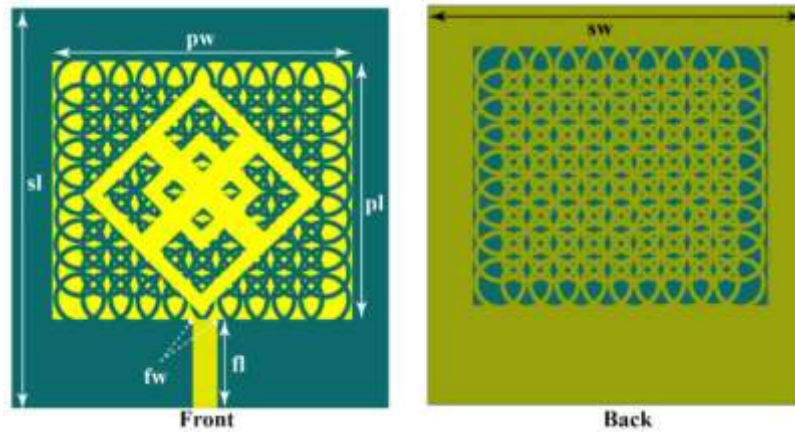
$$W = \frac{c}{2f} \times \sqrt{\frac{2}{\epsilon_r + 1}}$$

$$L = \frac{c}{(2f\sqrt{\epsilon_{eff}})} - 2 \times \Delta L$$

$$\Delta L = 0.412h \times \frac{\frac{\epsilon_{eff} + 0.3}{\frac{W}{h} + 0.264}}{\frac{\epsilon_{eff} - 0.258}{\frac{W}{h} + 0.8}}$$

In this context, the symbols λ for wavelength, c for speed of light, ' f ' for frequency, ϵ_r for dielectric constant, and ϵ_{eff} for the Effective Dielectric Constant are all used to indicate the following quantities.

Figure 3: Upper and lowest outlook of the SEA.



The construction of the patch consists of two centrally positioned rectangular frames that aim to improve radiation characteristics and optimize certain features such as bandwidth and gain. Furthermore, the patch has been designed with many symmetrical circular slots, which, when combined to form a complex pattern, enhance the antenna's radiation characteristics and bandwidth by maximizing current dispersion on the patch surface. An efficient energy transfer mechanism is provided by a short feed-line that spreads from the lowest of the patch and connects the antenna to the signal source. An antenna's gain and bandwidth can be enhanced by purposefully including a faulty slot on the ground plane side, which helps shape the radiation pattern. Additionally, the ground plane displays a complicated repeating lattice pattern that could improve the ground structure's electromagnetic characteristics, lowering loss and increasing performance metrics such as the reflection coefficient. The selection of materials

enhances the antenna's performance; copper's reliable grounding properties ensure efficient operation, while graphene's superior conductivity amplifies signal radiation. The antenna can accommodate future 6G applications due to its $100 \times 100 \mu\text{m}^2$ overall dimensions and $55 \times 70 \mu\text{m}^2$ patch area.

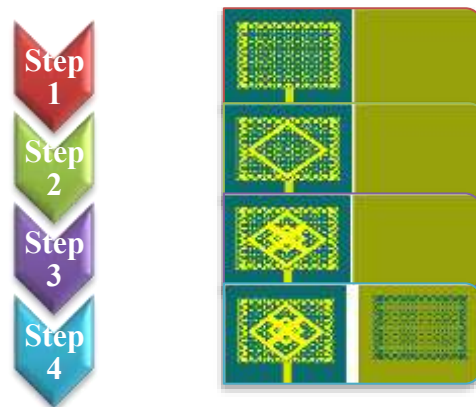
A number of antenna properties, comprising gain, bandwidth, and reflection coefficient, are being enhanced by these design modifications. Afterwards, they move on to model the antenna with the help of CST software. "The return loss, radiation pattern, and gain of the antenna" can be examined and studied in this stage. The antenna's behavior under various operating situations and frequencies can be better understood by modeling it.

2.2 Development of the single-element antenna

Figure 4 depicts the four main phases of the SEA's evolution, each of which is characterized by incremental improvements made in order to achieve peak performance. At the beginning of the design process, there is a rectangle patch element with round holes all over it. The circular slots are designed to improve the antenna's performance by affecting its resonant behavior. However, there are critical performance areas where it falls lacking. These limits make it clear that the design needs more work.

After the initial stage's difficulties are addressed, the design moves on to the second stage, which involves inserting a rectangular frame in the patch's center and encircling the circular slot pattern. The goal of this modification is to increase the antenna's gain and resonance. Based on the outcomes of the simulations, this revised design is an improvement over the original. However, more adjustments are required to achieve the desired parameters because the bandwidth and gain are still insufficient, even after these enhancements. Now they can go on to the next phase of the design process, where they are going to examine at more enhancements.

Figure 4: The development of improved SEAs



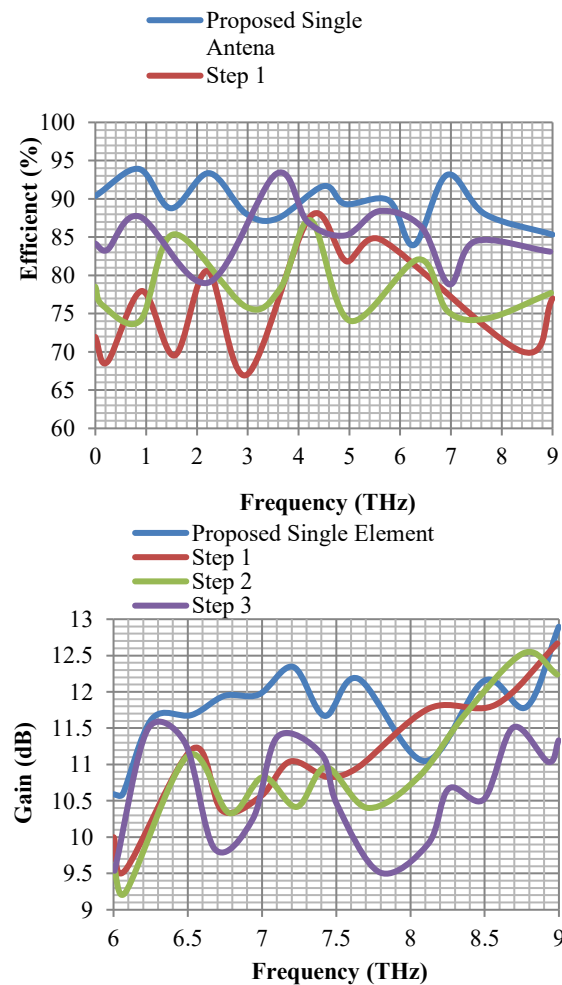
Substantial changes are performed to the patch element in the third stage of design development to further enhance its performance. In order to get better resonance properties, a more complicated geometry is created by establishing a second rectangular frame in the middle of the patch. After making these changes and running the simulations again, researchers see significant improvements. In particular, three separate resonance frequencies are attained in this design iteration. These improvements are certainly an improvement over the previous stage, but there is still opportunity for improvement as the return loss and bandwidth are virtually same.

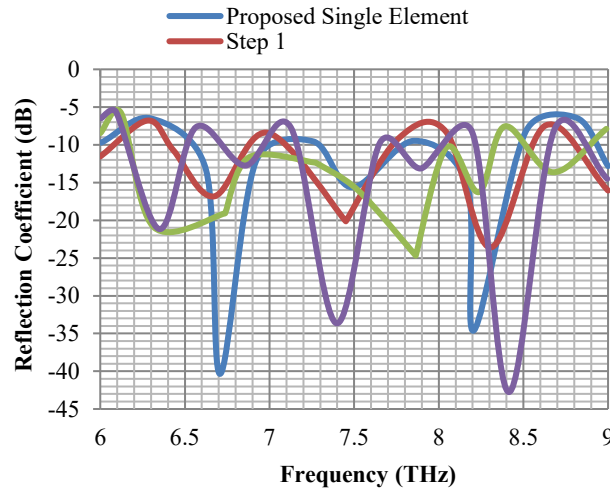
To solve the remaining problems with bandwidth and gain, a crucial improvement is implemented in the last step of antenna design development. This enhancement entails

the strategic incorporation of an unreliable ground slot, which dramatically modifies the antenna's ground plane.

The conceptual layout of the SEA undergoes a series of iterative modifications and optimizations, progressing from a basic configuration to a complex optimized structure that meets all performance requirements. The design process is fundamentally iterative, with each stage building upon insights from previous iterations to achieve the final goal. The figure 5 shows the performance indicators of the expansion of the single element antenna design in three iterative steps, which ends with the proposed final design. The efficiency graph indicates that the single element antenna proposed occupies the highest efficiency, always larger than 85% within the entire frequency range 0 to 9 THz, better than the Step 1, Step 2, and Step 3 which have lower and oscillating efficiencies. The gain plot shows that the improvement in gain is intended as the design moves on, with the proposed design attaining a gain peak of approximately 12.8 dB, at frequencies close to 9 THz, which suggests increased signal directionality and radiation characteristics. The obtained reflection coefficient (S11) results demonstrate that the suggested antenna has greatly improved impedance matching, especially at 6.8 THz and 8.5 THz, where S11 is less than -30 dB, reducing power reflection and improving total performance.

Figure 5: SEA Performance Metrics: (a) Gain, (b) Efficiency, and (c) S11

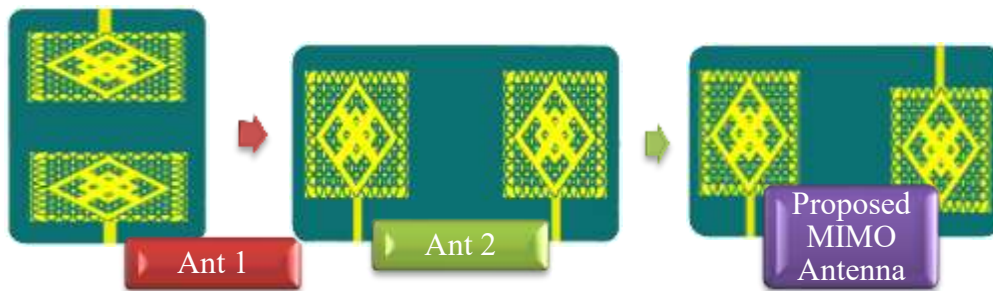




2.3 MIMO Antenna Devices

The next section provides illustrations of the graphene microstrip MIMO patch antennas. Researchers show how to build a two-port MIMO configuration from the ground up, building on the SEA, in the design methodology. This configuration improves signal reception in many ways, including “spatial diversity, interference mitigation, capacity enhancement, multipath exploitation, and strengthened security” [31]. As a first step in designing the best MIMO antenna, researchers must ascertain the ideal orientation of the antenna parts to obtain the necessary level of isolation. The antenna design made use of three different configurations, as shown in Figure 6. To ensure consistency in performance, the patch and ground structure were chosen to match those of the SEA.

Figure 6: Examining the three different MIMO antenna layouts, (a) Ant 1; (b) Ant 2; and (c) Ant 3 (Proposed)

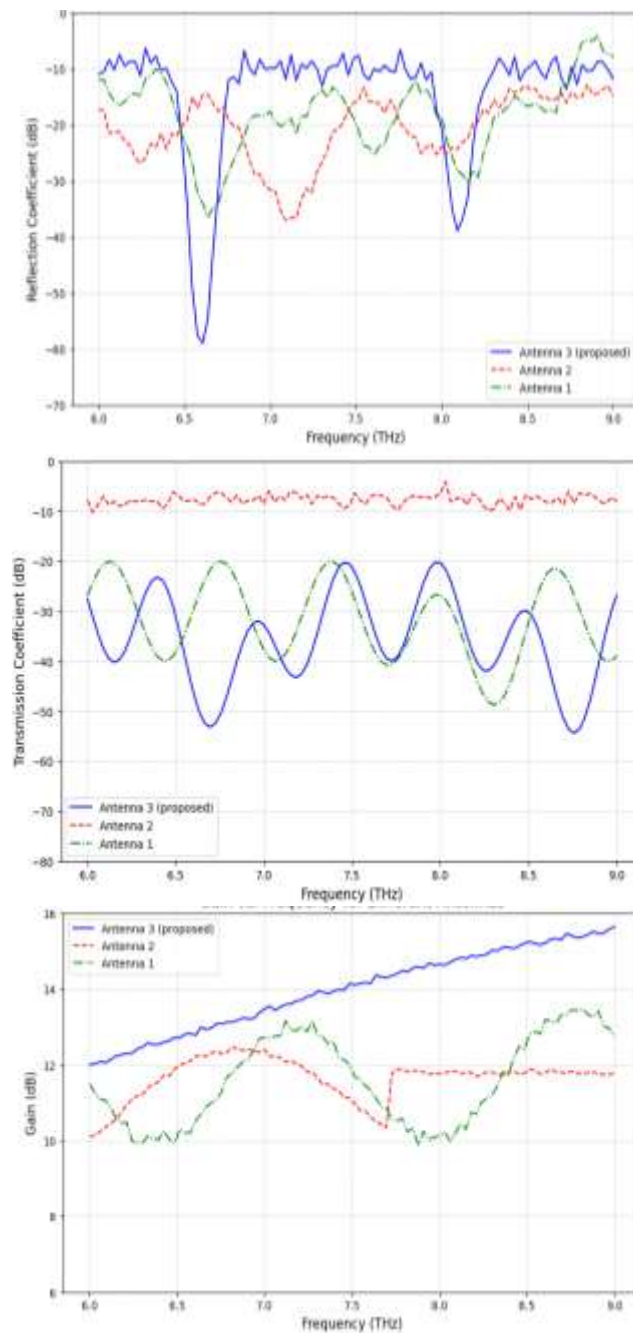


In all configurations, the edge-to-edge difference remains at 140μm, which allows for the antenna components to be properly spaced and aligned. As seen in Figure 6a, the first element is positioned side by side with the two elements in the first configuration (Ant. 1), which has a 0-degree orientation. In the second configuration (Ant. 2), seen in Figure 6b, the two pieces are positioned at 180 degrees, essentially inverted in relation to the first element. Figure 6c depicts the last possible arrangement (Ant. 3), which positions the two components perpendicular to one another and 180 degrees from the initial element.

The comparative analysis of the performance of the 3 MIMO antenna configurations, Antenna 1, Antenna 2, and the proposed Antenna 3, proves significant improvements in reflection coefficient (S11), transmission coefficient (S21), and gain (as seen in Figure 7). The S11 plot indicates that Antenna 3 obtains a deep resonance of almost -65 dB at

around 6.5 THz, outperforming Antenna 1 and Antenna 2, which still plot between -15 and -30dB. The S21 readings show tighter isolation for Antenna 3 ranging from -20 to -60 dB, whereas Antenna 1 shows about -10 dB and Antenna 2 in the -15 to -30 dB range. With respect to gain, Antenna 3 is always higher, rising from approximately 12 dB at 6 THz to almost 16 dB at 9 THz, whereas Antenna 2 stays around 11-12 dB, and Antenna 1 oscillates between 9-13dB. This verifies Antenna 3's increased efficiency and isolation.

Figure 7: Examining the Three Different MIMO Antenna Setups: (a) S11, (b) S21, and (c) Gain



2.4 Diversity Parameters for MIMO Antenna

Some diversity parameters are employed to assurance the quality of a MIMO antenna, alongside S-parameters and radiation characteristics. In order for MIMO antennas to be used in real-world scenarios, the diversity parameters must have predetermined values. Therefore, some basic diversity features of MIMO antennas are covered in this section.

a) Envelope Correlation Coefficient (ECC)

ECC is an essential metric in MIMO antenna design, assessing the correlation between radiating elements. A lower ECC value, ideally close to zero, signifies excellent isolation and minimal signal correlation, thereby enhancing diversity gain, system capacity, and overall performance in modern wireless communication systems [32]. Equation (1) provides the measured equation for ECC:

$$ECC_{qp} = \frac{\left| \int_0^{2\pi} \int_0^\pi (E_{\theta p}^* E_{\theta q} P_{\theta}^{XP} + E_{\phi p}^* E_{\phi q} P_{\phi}) \right|^2}{\alpha \times \beta} \quad (1)$$

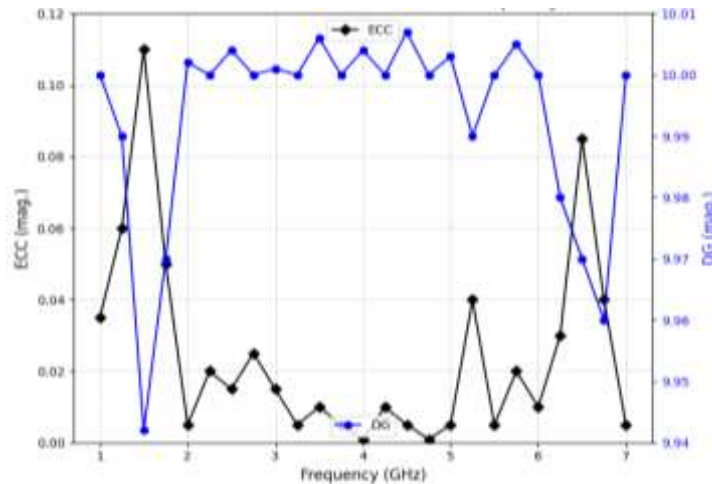
b) Diversity Gain (DG)

It is as significant parameter in MIMO antenna systems that measure the development in signal reception due to diversity techniques. An advanced DG value specifies better reliability, reduced fading effects, and enhanced overall performance of wireless communication systems. Equation (2) [33] could be used to determine the DG by utilizing the ECC value:

$$DG = 10 \times \sqrt{1 - |ECC_{qp}|^2} \quad (2)$$

Figure 8 shows the performance of an antenna system by measuring ECC and DG as frequency increases. The ECC measures how independent the elements of an antenna system are; therefore, lower ECC values give better performance. The ECC is below 0.03 within the range of approximately 2.25 GHz to 5.0 GHz and increases to 0.04 at 5.25 GHz and over 0.08 at 6.75 GHz. DG gives a measure of the increase in signal-to-noise due to diversity performance. The DG is high throughout the frequency range, approximately 10.0 dB. Where the ECC spikes at 1.5 GHz and shows a peak at 6.5 GHz, the diversity gain drops to approximately 9.94 dB and 9.96 dB, respectively, indicating a slight decrease in expected performance at these frequencies. Overall, the antenna is shown to have stable performance in the 2.25 GHz to 6.75 GHz band, along with high diversity gain and low correlation across a good bandwidth.

Figure 8: Simulated ECC and DG characteristics of MIMO Antenna



c) Channel Capacity Loss (CCL)

It is the highest level of data transmission across a communication channel at which almost no loss occurs. For each particular MIMO system, the predetermined CCL value is less than 0.4 bits/s/Hz. Equation (3) give the expressed value of CCL when S-parameters are used [34]:

$$CCL = -\log_2 \det (\vartheta^\mu) \quad (3)$$

Wherever

$$\vartheta^\mu = \begin{bmatrix} \xi_{11} & \xi_{12} \\ \xi_{21} & \xi_{22} \end{bmatrix} \quad (4)$$

Then

$$\begin{aligned} \xi_{11} &= 1 - [|S_{11}|^2 + |S_{12}|^2] \\ \xi_{12} &= -[S_{11}^* S_{12} + S_{21}^* S_{12}] \\ \xi_{21} &= -[S_{22}^* S_{21} + S_{12}^* S_{21}] \\ \xi_{22} &= 1 - [|S_{22}|^2 + |S_{21}|^2] \end{aligned}$$

d) Total Active Reflection Coefficient (TARC)

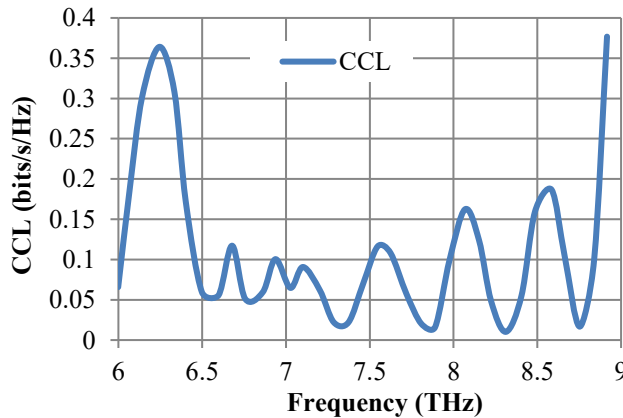
In a MIMO system, TARC is the ratio of the patch's incident power to the overall reflected power from the radiating components. Equation (5) [35] gives the formula for the modified TARC for a 2-port MIMO antenna:

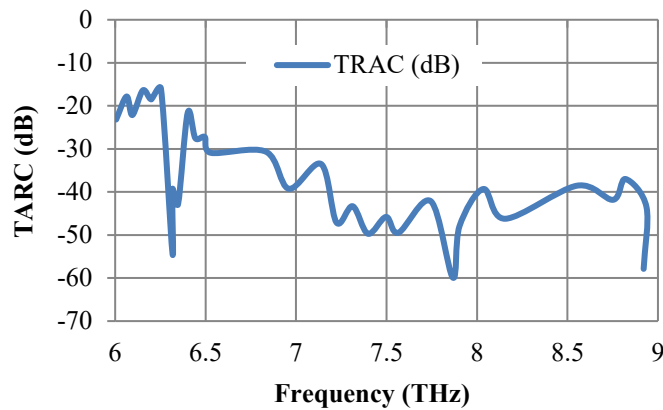
$$TARC = \sqrt{\frac{|S_{11} + S_{12} e^{j\theta}|^2 + |S_{21} + S_{22} e^{j\theta}|^2}{4}} \quad (5)$$

It is anticipated that the antenna can absorb all of the power, as the TARC is calculated as the ratio of incident power to reflected power. Therefore, zero is the optimal TARC value for a MIMO antenna.

Figure 9 shows the simulated performance of a MIMO antenna over a frequency band of 6 THz to 9 THz in two important measures, CCL and TARC. The CCL is the loss of channel capacity as a result of signal correlation. It is also low, typically less than 0.2 bits/s/Hz, in most of the band, with significant exceptions of 0.36 bits/s/Hz at about 6.25 THz and other highs around 0.2 bits/s/Hz at 8.75 THz. A lower CCL is desired. The TARC quantifies the mutual coupling and overall antenna mismatch. This figure is consistently small (less than -20 dB) throughout the frequency range with major dips to around -50 dB at 7.5 THz and -60 dB at 8 THz. Such low TARC values imply high-quality impedance equivalence and low signal reflection that are important to effective operation of MIMO antennas.

Figure 9: Simulated CCL and TRAC characteristics of MIMO Antenna

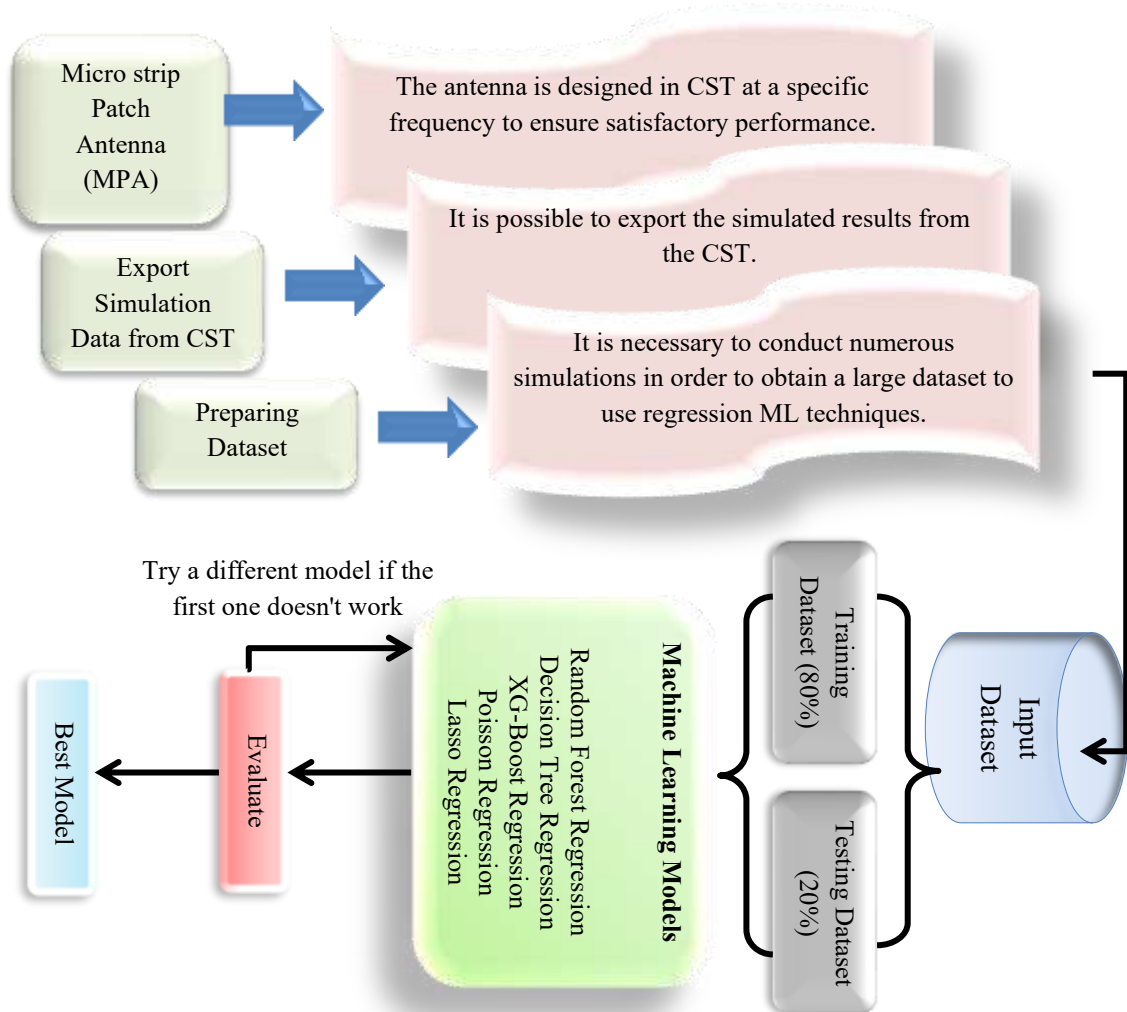




2.5 Machine Learning Model

Figure 10 illustrates a structured workflow for designing, simulating, and optimizing a Microstrip Patch Antenna (MPA) using CST software in combination with ML techniques for performance prediction. The process begins with the design of the microstrip patch antenna in CST, where the antenna is tuned at a specific frequency to ensure satisfactory performance.

Figure 10: Schematic depicting the steps required to develop ML



Once the design is completed, the simulation data (such as bandwidth) is exported from CST for further analysis. Since ML models require large datasets to achieve high accuracy, a dataset is prepared by performing repeated simulations, thereby generating sufficient input-output pairs for training and testing. This dataset is divided into two subsets: 80% for training and 20% for testing. The training dataset is then used to train various ML regression models, which include "Decision Tree Regression, XG-Boost Regression, Random forest regression, Poisson Regression, and Lasso Regression". After training, the methods are evaluated using the testing dataset to measure their accuracy and error. If the accuracy of a chosen model is not satisfactory, another regression model is applied. The model that demonstrates the greatest performance in terms of prediction accuracy and minimal error is selected as the best model. Finally, this best-performing model is used to make reliable predictions about antenna performance without requiring further CST simulations, thereby saving computational resources and design time.

a) Decision tree regression

It is a subset of regression analysis that uses decision trees as its predictive model. Typically, decision trees are employed to address classification issues; however, by modifying the trees, regression problems could also be addressed [36].

b) Random forest regression (RFR)

One ML approach called RFR attempts to predict a continuous target variable using a collection of input features. It is mostly used for classification issues and is an offspring of the popular RF method; it is a member of the ensemble learning family [37].

c) XGB regression

It is a famous and very successful ML created by combining decision trees using XGBoost, a ML algorithm. The efficacy, ability to manage big datasets, and competitive performance in ML contests have contributed to its widespread use and increased visibility in the field [38].

d) Poisson regression (PR)

In regression analysis, PR is used when the dependent variable is a count and the counts are assumed to follow a Poisson distribution. This method is commonly used when the dependent variable represents the frequency of occurrences within a specified time or location period [39].

e) Lasso regression

The "Least Absolute Shrinkage and Selection Operator" (LASSO) regression technique incorporates a penalty component into the ordinary least squares (OLS) target function. It is a linear regression approach. Researchers find that this penalty factor is inversely related to the absolute values of the regression coefficients. Lasso regression typically tries to set certain coefficients to zero in order to improve model sparsity, which is its major purpose. This can be particularly useful when dealing with datasets that contain a large number of features, as it executes feature selection [40].

2.6 Performance measurement metrics

ML models are evaluated for accuracy and efficacy using performance assessment measures. Researchers intend to employ the following statistical measures to evaluate these models: "R-squared (R²), Mean Squared Error (MSE) [43], Explained Variance Score (Var Score) [45], Mean Absolute Error (MAE) [41], and Root Mean Squared Error

(RMSE) [42]". Each measure serves a specific function, and the choice is dependent upon the aims of the regression analysis. MAE and RMSE evaluate the average magnitude of errors, while R-squared and Explained Variance Scores provide insights into the variability eliminated by the model [46].

$$MAE = \frac{1}{n} \sum_{i=1}^n |y_i - \hat{y}_i|$$

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

$$RMSE = \sqrt{MSE}$$

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

$$\text{Explained variance } (y, \hat{y}) = 1 - \frac{Var(y - \hat{y})}{Var(\hat{y})}$$

3. Result and Discussion

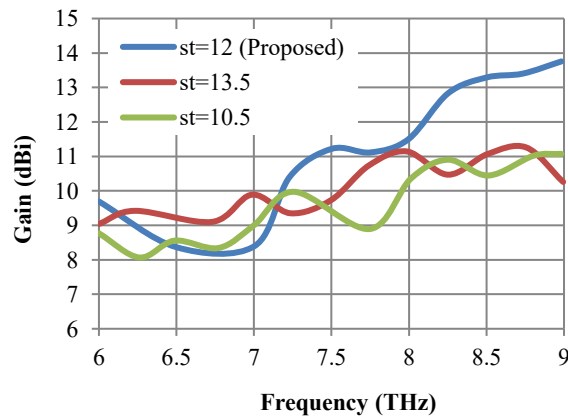
3.1 Parametric analysis

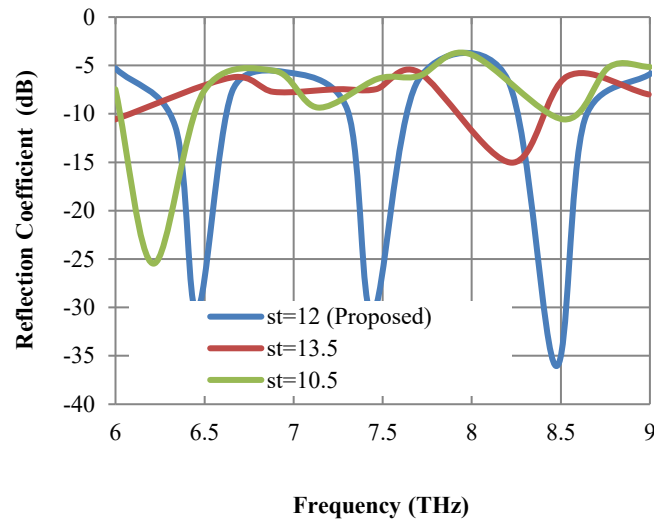
Parametric analysis is an important tool in antenna design since it allows one to examine the impacts of changing certain parameters on the antenna's performance. Antenna engineers can discover a lot about the effects of changing dimensions, materials, or configurations on important metrics including radiation characteristics, return loss, and bandwidth through experimentation.

a) Substrate thickness (St)

The design parameter that is vital in antenna design is substrate thickness (st), which is the physical thickness of the dielectric layer between the radiating patch and the ground plane. It has a direct influence on such important performance parameters of the antennas as gain, bandwidth, and impedance matching. The influence of the different substrate thicknesses (st = 10.5 μm , 12 μm (proposed), and 13.5 μm) on the antenna performance is tested in the given figure 11. As can be seen, the gain graph indicates that the gain is highest with st = 12 μm and attains approximate 13.8dBi at 9 THz, in contrast to the gain attainable with st = 13.5 μm (approximately 11.2dBi) and 10.5 μm (approximately 11.0dBi). The reflection coefficient (S11) plot shows better matching impedance in the proposed design, with deepest minima at -30 dB at 6.8 THz and 8.5 THz, and other thicknesses exhibit higher values of S11, signifying higher signal reflection.

Figure 11: Efficiency variations as a function of st (a) Gain, (b) Reflection coefficient

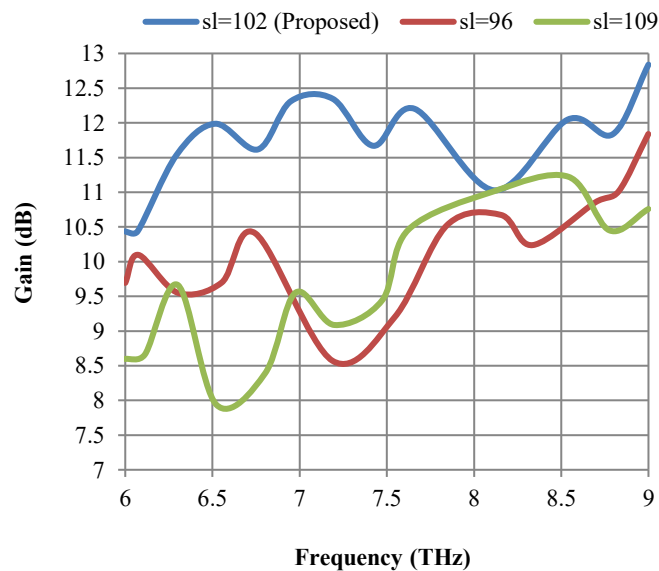


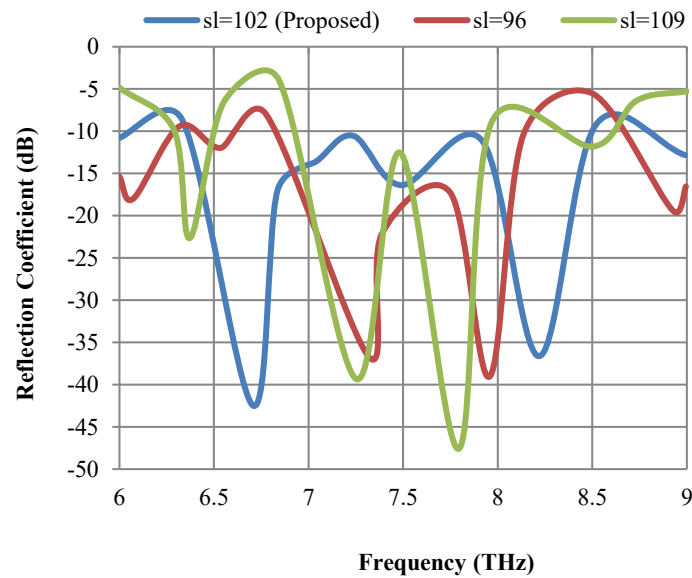


b) Substrate Length (sl)

It is the physical length of the dielectric layer below the antenna patch that has a major impact on the electromagnetic properties of the “antenna, gain, bandwidth and impedance matching”. The influence of the different lengths of the substrate ($sl = 96 \mu\text{m}$, $102 \mu\text{m}$ (proposed), and $109 \mu\text{m}$) on the results of the antenna performance is studied in the figure 12. As shown in the gain graph, the maximum gain is obtained at $sl = 102 \mu\text{m}$ (maximum gain of about 12.8dBi at about 9 THz), followed by $sl = 96 \mu\text{m}$ and $sl = 109 \mu\text{m}$, which attain gain of about 11.0dBi and 11.2dBi, respectively. The reflection coefficient (S11) curve demonstrates that the proposed design has better impedance match with deep minima of less than -40 dB at frequencies below 6.8 THz and 7.8 THz. Other substrate lengths, on the contrary, have a shallower S11 dip, which indicates greater signal reflections and worse performance.

Figure 12: Efficiency variations as a function of sl (a) Gain, (b) Reflection coefficient

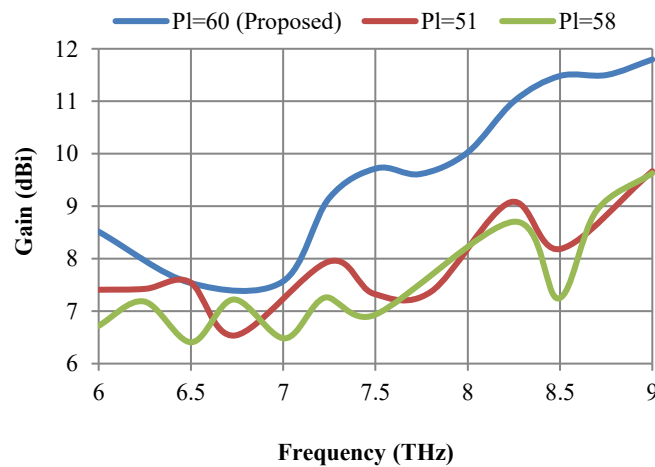


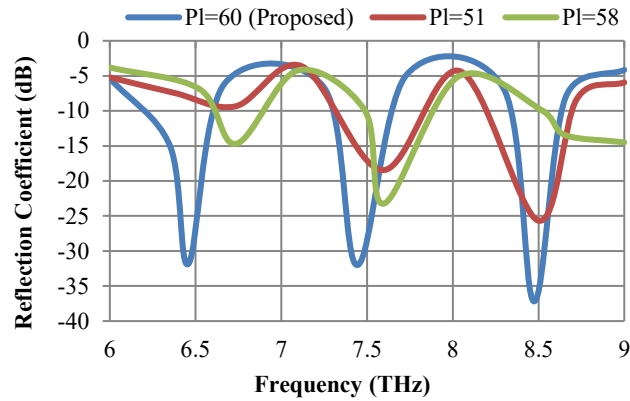


c) Patch Length (pl)

Patch length (pl) refers to the actual length of the radiating patch in an antenna. This dimension plays an important role in gain, bandwidth, and impedance matching. The results shown in the figure 13 analyze the effect of different patch length (pl = 51 μm , 58 μm , and 60 μm (proposed)) on the antenna. The gain graph shows that the proposed patch length (pl = 60 μm) achieved the maximum gain of about 11.8 dBi at 9 THz, while the pl = 51 μm and pl = 58 μm had a gain of about 9.0 dBi and 9.5 dBi, respectively. For the reflection coefficient (S11) graph, the reflection coefficient improved towards impedance matching, at the same frequencies, pl = 60 largest minima approximately equal to deep -30 dB at frequencies somewhat near 6.8 THz and at about 8.5 THz. The other patch lengths of 51 μm and 58 μm had shallower minima, suggesting poorer matching and increased power reflection, reinforcing that patch length is an important design optimization parameter.

Figure 13: Effects of changing the length of the patch on the gain and reflection coefficient of an antenna





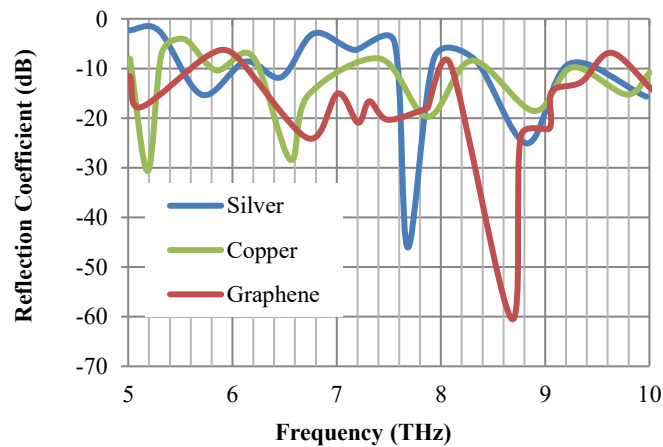
d) Patch analysis

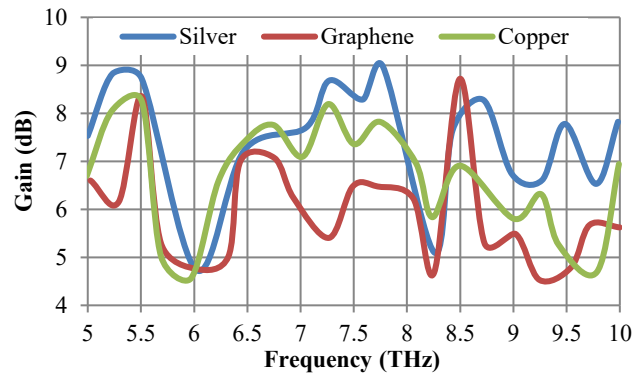
The high conductivity of silver, graphene, and copper prompted their evaluation as patch and ground components to improve antenna performance for THz applications. An exhaustive investigation was conducted to determine the best mix of materials to achieve exceptional performance. The final material choice and the measures used to evaluate it are detailed in this section.

• Surface Material Variation Using a Fixed Copper Patch Element

Figure 14 depict the impact of different ground materials—copper, graphene, and silver—on antenna performance with a constant copper element in reflection coefficient (S11) and gain within the 5–10 THz range. In the S11 response, graphene has the strongest resonance, dropping close to -60 dB at 8.7 THz, followed by drops below -30 dB at 6.2 THz and 9.5 THz. Silver has moderate reflectance, approximately -15 to -25 dB for most frequencies, while copper has several resonances, falling to almost -30 dB at 6 THz. Silver is the best and most stable gain in terms of magnitude, with a value of over 9 dB at 5.5 THz, holding values greater than 7 dB for several bands. Copper indicates moderate gain (6–8 dB), whereas graphene varies between 5–8.5 dB with the maxima around 8.5 THz. Graphene improves impedance matching, silver improves gain, and copper balances both factors.

Figure 14: Impact of several types of ground on the performance of a fixed-element antenna: (a) S11; (b) gain

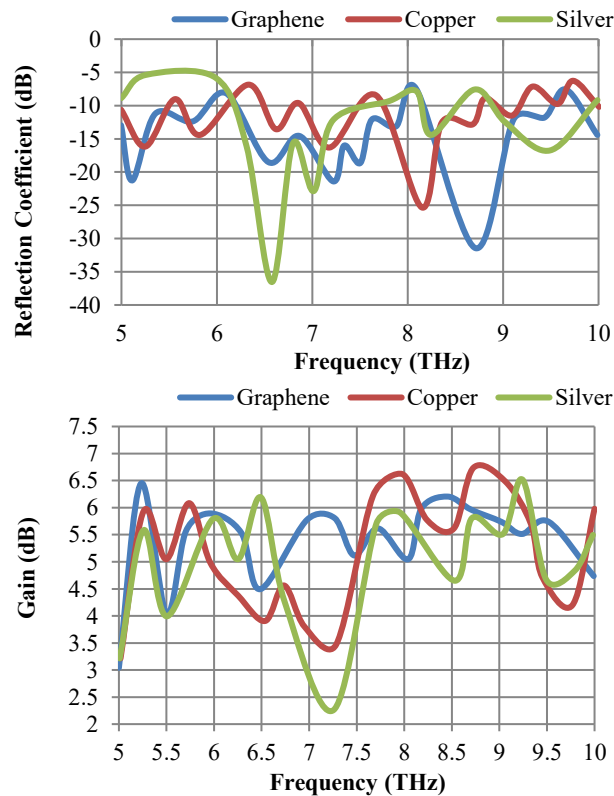




• **Surface Material Variation Using a Fixed Silver Patch Element**

Figure 15 of the given parameters show how different ground materials, which are graphene, copper and silver, can influence the functioning of the antenna at fixed silver element. Plot S11 demonstrates that graphene offers deeper reflection minima and more stable minima, which suggests a high impedance matching as compared to copper and silver with sharp dips at 6.5 THz. The gain plot indicates that copper has always higher values of peak gain that are greater than 6.5 dB at several frequencies, whereas graphene and silver have moderate and stable gain and lower and more variable respectively. In general, graphene is impedance-matching, copper is gain-enhancing, and silver is selectivity-frequency-benefiting, demonstrating material-related antenna performance trade-offs.

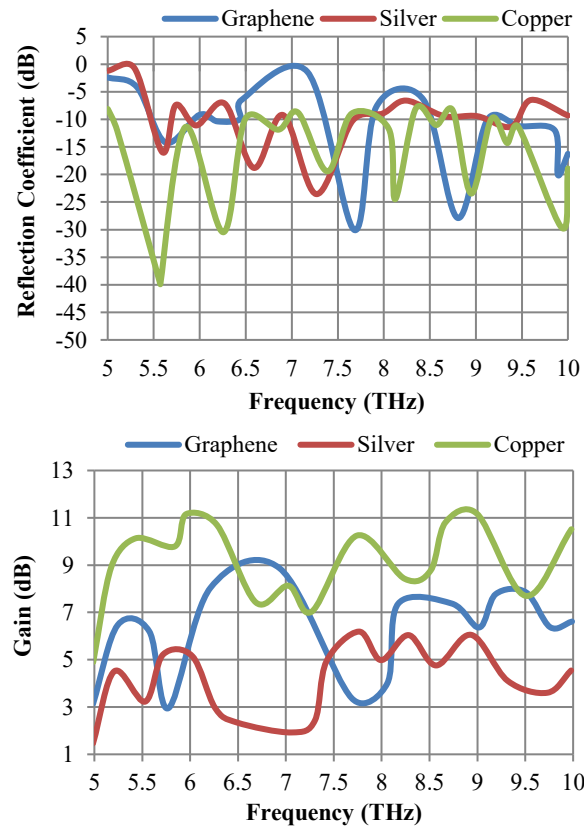
Figure 15: Antenna performance with a fixed silver element and the effect of ground material variation: (a) S11; (b) gain



• **Material Variation Including a Fixed Graphene Patch Element**

Figure 16 indicate the effect of various ground materials—graphene, silver, and copper—on antenna performance with a constant graphene element in terms of reflection coefficient (S11) and gain in the 5–10 THz frequency range. The S11 data indicate that graphene has deeper minima in reflection, which amounts to approximately -25 dB at 7 THz and -20 dB at 9 THz, resulting in improved impedance matching. A copper display steep dips below -35 dB at 5.8 THz and 9.7 THz, showing very strong resonances, whereas silver is relatively shallow, typically -10 dB. The gain plot is pointing towards copper's better performance, recording above 11 dB near 6.5 THz and 9 THz, while graphene has moderate gain of 6–8 dB. Silver runs weakest, with gain largely 2–6 dB. Generally, graphene maximizes impedance matching, copper maximizes gain, and silver demonstrates minimal improvements.

Figure 16: Impact of several types of ground on the performance of a fixed-graphene antenna: (a) S11; (b) gain

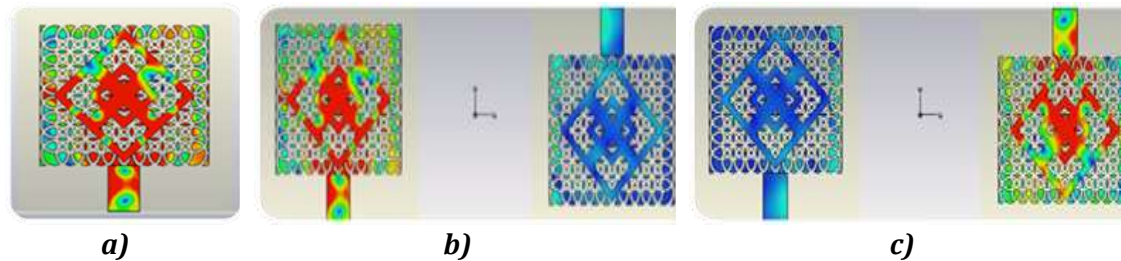


e) Surface current

An antenna current distribution shows the current distribution along the conducting elements of an antenna. This distribution has a significant impact on the radiation pattern of an antenna, which is its ability to send and receive electromagnetic signals. At 6 THz, the surface distribution of current for a single element achieves its maximum value of 22310.8 A/m, as shown in Figure 17a. Flows around the feed-line and centre frame provide the strongest surface currents in the patch. An MIMO antenna with a single stimulated port and loads radiating from the other ports could be shown in Figure 17b, which depicts the predicted distribution of surface currents. If the surface current that triggers Ant.1 is eliminated, then no antenna in Figure 17c can detect a surface

current. The remaining antennas do not generate surface current, with the exception of Antenna 2, as seen in Figure 17c.

Figure 17: Surface Current (a) Antenna with a Single Element; (b) Antenna with Multiple Inputs and Outputs (MIMO) at port 1; and (c) Such an antenna at port 2



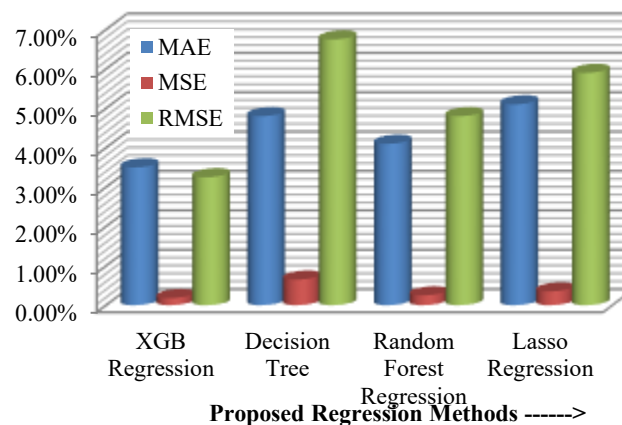
3.2 Regression ML Model Analysis

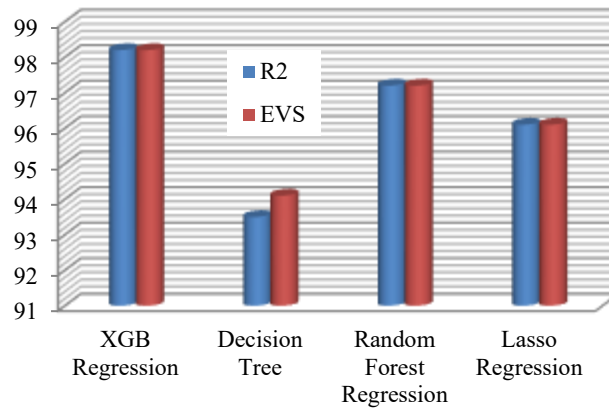
Table 2 outlines the comparative analysis of various regression algorithms for gain prediction performance using evaluation metrics such as “MAE, MSE, RMSE, R^2 , and EVS”. Out of all the regression algorithms evaluated, XGB Regression provides the best overall performance, with generally lower errors (MAE: 3.50%, MSE: 0.18%, RMSE: 3.25%), and the strongest explanatory capability (R^2 and EVS = 98.20%). Random Forest Regression follows closely with slightly higher errors and strong R^2 (97.20%) and EVS (97.50%) scores. Decision Tree Regression is comparable but with less optimal errors than Random Forest (MAE: 4.80%, RMSE: 6.75%) and only R^2 at (93.50%). Lastly, when applied, Lasso Regression had the worst results in terms of gain prediction performance among the models considered, producing the highest errors (MAE: 5.10%, RMSE: 5.90%) at the same time still achieving good R^2 and EVS values of 96.10%. Figure 18 presents the comparison graph of gain prediction performance.

Table 2: The accuracy of the gain predicted

Algorithm	MAE	MSE	RMSE	R^2	EVS
XGB Regression	3.10%	0.18%	3.25%	98.20%	98.20%
Decision Tree	4.80%	0.65%	6.75%	93.50%	94.10%
Random Forest Regression	4.10%	0.25%	4.80%	97.20%	97.50%
Lasso Regression	5.10%	0.35%	5.90%	96.10%	96.10%

Figure 18: Comparison bar Chart for Performance





Proposed Regression Methods ----->

Table 3 presents a comparison between different machine learning models that are implemented in antenna design using performance measures. Past research conducted with a Random Forest Regression showed mixed results with one study attaining low MAE of 3.15 whereas other study recorded very high of 86.1. Extra Tree Regression also demonstrated mixed results with one achieving MAE of 4.01 and the other way higher of 4.50. By comparison, XGB Regression has the lowest MAE (3.10%), MSE (0.18%), and RMSE (3.25%), and the highest R2 (98.20) and EVS (98.20), meaning it is more accurate and predicts better generalization of the antenna design.

Table 3: Using performance measurements compare ML models for antenna design

[Reference]	Models	MAE	MSE	RMSE	R2	EVS
[26]	Random Forest Regression	3.15	0.3	4.51	95.51	96.62
[47]	Random Forest Regression	86.1	38.16	5.72	82.6	97.47
[48]	Extra Tree Regression	4.01	0.22	4.71	97.71	97.71
[17]	Extra Tree Regression	4.50	7.01	8.45	82.13	85.68
Our Work	XGB Regression	3.10%	0.18%	3.25%	98.20%	98.20%

4. Conclusion

In the research, the authors were able to show the design and optimization of a compact and high-performance MIMO antenna system optimized towards 6G terahertz (THz) communication systems. The proposed antenna-based on the use of advanced materials like graphene patch and copper ground plane together with a polyimide substrate resulted in outstanding electromagnetic characteristics. The ML models were used to optimize the performance of the antennas, whereby XG-Boost regression reported the best results: R 2 of 98.20, MAE of 3.10, MSE of 0.18, and RMSE of 3.25. The results validated very precise gain, bandwidth and isolation predictions, saving much time in simulating CST repeatedly.

The optimized MIMO antenna had two band resonances with a peak gain of 13.8dBi at 9 THz, isolation of over -65 dB, and efficiency of more than 85. Moreover, the diversity performance was good with ECC being less than 0.03 and DG being constant at a broad

bandwidth of about 10dB. The design was also confirmed to be accurate by RLC circuit modeling and ADS simulations, which both simulated to give similar reflection coefficient (S_{11}) values. The scope in the future entails increasing the AI models to real-time adaptive optimization, investigating novel meta-materials to enhance miniaturization, and incorporating reconfigurable antenna designs to enable dynamic 6G spaces.

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