

# DESIGN AND ANALYSIS OF 2-D PIN PHOTODIODE USING MoS<sub>2</sub>

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**Abstract:** In the project 'Design and Analysis of Capacitive Accelerometer,' the focus was on evaluating The integration of two-dimensional materials, such as molybdenum disulfide (MoS<sub>2</sub>), into semiconductor devices has attracted significant attention due to their unique electronic properties and potential for low-power electronics. This research focuses on simulating a PIN (p-type/intrinsic/n-type) photodiode structure using MoS<sub>2</sub> as the intrinsic layer for applications requiring low frequency and low power consumption. The objective is to investigate the feasibility of MoS<sub>2</sub>-based PIN photodiodes and analyse their performance characteristics through numerical simulations. The study aims to contribute insights into the optimization of next-generation photodiode devices for emerging electronic applications.

The demand for energy-efficient electronic devices with reduced power consumption and operational frequencies has driven researchers to explore novel materials and device architectures. Among these materials, two-dimensional semiconductors like molybdenum disulfide (MoS<sub>2</sub>) have emerged as promising candidates for low-power electronics due to their unique electronic properties and scalability. In this study, we focus on simulating a PIN (p-type/intrinsic/n-type) photodiode structure utilizing MoS<sub>2</sub> as the intrinsic layer. The PIN diode configuration is well-suited for applications requiring low frequency and minimal power consumption, making it ideal for sensor networks, wearable devices, and Internet of Things (IoT) applications. The simulation process involves modelling the MoS<sub>2</sub>-based PIN photodiode using numerical simulation tools to predict its electrical characteristics under various operating conditions. Parameters such as carrier mobility, bandgap energy, and responsivity are considered to optimize the device performance for low-frequency operation.

In conclusion, the simulation of a PIN photodiode using MoS<sub>2</sub> material holds great promise for advancing the field of low-power electronics and optical sensing. This research represents a critical step towards developing efficient and compact photodiode devices that can meet the growing demand for energy-efficient electronic systems in various industries.

**KEYWORDS:** COMSOL Multiphysics, Diodes, Optical Power, Bandgap, Electrical Field, MoS<sub>2</sub>, GaAs.

## 1. INTRODUCTION

### 1.1 PROBLEM STATEMENT

#### Simulation of PIN Photodiode with MoS<sub>2</sub> Material for Low Frequency and Low Power Applications

In recent years, there has been a growing demand for semiconductor devices capable of operating at lower frequencies and consuming minimal power, particularly in the field of wireless communications, sensor networks, and Internet of Things (IoT) devices. Traditional PIN diodes, while versatile and widely used in high-frequency applications, may not be optimal for low-power and low-frequency applications due to inherent limitations in material properties and device design.

The advancement of semiconductor technology has led to the exploration of new materials and device architectures aimed at achieving enhanced performance and efficiency, particularly in low-frequency and low-power applications. In this context, the simulation of

- PIN (Positive-Intrinsic-Negative) diode using molybdenum disulfide ( $\text{MoS}_2$ ) as the semiconductor material presents an intriguing research opportunity. The primary challenge addressed by this project is the investigation of the feasibility and performance characteristics of  $\text{MoS}_2$ -based PIN diodes under conditions relevant to low-frequency and low-power electronic systems.

Traditional PIN diodes, composed of silicon or gallium arsenide, have established roles in high-frequency applications such as RF switches and detectors. However, their performance at lower frequencies and power levels may be suboptimal due to inherent material properties and limitations. By leveraging the unique properties of  $\text{MoS}_2$ , including its two-dimensional layered structure, direct bandgap, and high carrier mobility, we aim to design and simulate PIN diodes that are specifically tailored for low-frequency operation with minimal power consumption.

## 1.2 OBJECTIVE

- The main objective of this project is to design a 2-D (Two – Dimensional) PIN Photodiode using the material  $\text{MoS}_2$  (Molybdenum Disulfide).
- Compare the performance of the  $\text{MoS}_2$ -based PIN diode with conventional semiconductor materials like GaAs (Gallium Arsenide).
- The PIN Photodiode sensor is designed in COMSOL Multi-Physics 6.2v and we have compared with GaAs (Gallium Arsenide).
- The Characteristics of PIN Photodiode can be analysed with  $\text{MoS}_2$  (Molybdenum Disulfide) and GaAs (Gallium Arsenide) in terms of Electric Field Analysis, Bandgap Analysis (Spontaneous Emission), and Total Power Output with Incident radiation of Light.

## 1.3 MOTIVATION

The motivation behind simulating a PIN diode utilizing  $\text{MoS}_2$  material for low frequency and low power applications stems from the continuous pursuit of enhancing semiconductor device performance and exploring innovative materials for next-generation electronics. This research endeavor is fueled by several compelling factors that underscore the potential impact and significance of developing  $\text{MoS}_2$ -based PIN diodes in the realm of low-frequency and low-power electronics.

Firstly, the quest for energy efficiency in electronic devices has become increasingly imperative in recent years. Traditional semiconductor materials face limitations in terms of power consumption and operational frequencies, particularly in applications requiring low-power consumption and operation at frequencies below gigahertz ranges. By harnessing the unique properties of  $\text{MoS}_2$ , such as its high carrier mobility, low contact resistance, and tunable bandgap, we aim to develop PIN diodes that exhibit superior performance characteristics ideal for low-power applications.

## 2. LITERATURE SURVEY

### .1 EXISTING RESEARCH ON PIN DIODES AND $\text{MOS}_2$ -BASED

## DEVICES

PIN diodes and MoS<sub>2</sub>-based devices represent two distinct areas of semiconductor device research with significant implications for modern electronics. This literature review examines the current state of research on PIN diodes and MoS<sub>2</sub>-based devices, highlighting key findings, advancements, and future directions in these fields.

### 2.1.1 REVIEW OF EXISTING RESEARCH ON PIN DIODES

PIN diodes are semiconductor devices with a p-type, intrinsic, and n-type semiconductor structure, widely used in RF switching, photodetection, and other applications. Extensive research has focused on optimizing PIN diode performance, including reducing capacitance, improving linearity, and enhancing breakdown voltage.

Recent studies have explored novel materials and device architectures for PIN diodes, aiming to enhance efficiency and versatility. For example, research on III-V compound semiconductors and silicon-based PIN diodes has led to improvements in high-frequency performance and power handling capabilities. Additionally, advancements in fabrication techniques, such as epitaxial growth and ion implantation, have enabled the production of high-quality PIN diode structures with tailored properties.

Furthermore, the integration of PIN diodes into complex electronic circuits and systems has been a subject of interest, particularly in the development of integrated RF front-end modules for wireless communication and radar applications. Overall, existing research on PIN diodes underscores their importance in modern electronics and highlights ongoing efforts to optimize performance and expand their application scope.

### 2.1.2 REVIEW OF EXISTING RESEARCH ON MOS<sub>2</sub>-BASED

#### DEVICES

MoS<sub>2</sub> is a two-dimensional semiconductor material that has garnered significant attention for its unique electronic properties and potential applications in nanoelectronics. Research on MoS<sub>2</sub>-based devices, including field-effect transistors (FETs), photodetectors, and diodes, has demonstrated promising performance metrics for low-power and high-speed applications.

Studies have investigated the synthesis methods, defect engineering, and doping strategies to tailor the electronic properties of MoS<sub>2</sub>. For example, doping MoS<sub>2</sub> with certain elements can modify its bandgap and carrier mobility, enabling precise control over device characteristics. Moreover, the integration of MoS<sub>2</sub> with other materials, such as graphene or h-BN (hexagonal boron nitride), has led to hybrid device architectures with enhanced performance and stability.

Applications of MoS<sub>2</sub>-based devices in optoelectronics, flexible electronics, and quantum technologies have also been explored. Research efforts focus on scaling up production methods and developing reliable device fabrication processes to enable commercialization and widespread adoption of MoS<sub>2</sub>-based devices.

In summary, existing research on both PIN diodes and MoS<sub>2</sub>-based devices highlights ongoing advancements in semiconductor device technology and materials science. Future research directions may include exploring new materials, optimizing device performance, and integrating these technologies into next-generation electronic systems.

## 2.2 ROLE OF DIODE IN ELECTRONICS

In the intricate world of electronics, diodes play a fundamental and indispensable role, serving as key components that enable the flow of electric current in specific directions while blocking

it in others. A diode is a semiconductor device that exhibits a nonlinear current-voltage characteristic, allowing it to function as a one-way valve for electrical current within electronic circuits. This essay aims to explore the essential characteristics, operating principles, and diverse applications of diodes in modern electronics.

## DESIGN OF PIN PHOTODIODE BASED ON MoS<sub>2</sub> USING COMSOL MULTIPHYSICS

### COMSOL MULTIPHYSICS

COMSOL Multiphysics is a software package which is widely used for modelling. This software not only helps to define the geometry, meshing, defining physics but also helps to visualize the end results. The mathematical structure in COMSOL Multiphysics is a system of partial differential equations.

Using these applications modes, you can perform various types of analysis including.

5. Stationery and time-dependent analysis
6. Linear and non-linear analysis
7. Eigen frequency and modal analysis

When designing, COMSOL Multiphysics uses the proven Finite Element Method (FEM). MEMS module is a part of the COMSOL Multiphysics software. This module helps in designing any type of MEMS device and do further analysis.

### 3.1 COMSOL INTRODUCTION

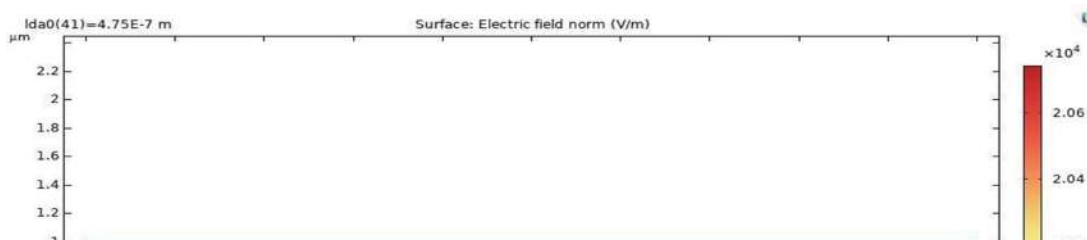
Here we use COMSOL Multiphysics Software.

COMSOL Multiphysics stands as a flagship platform in the realm of Multiphysics simulation and modeling. At its core, it's a versatile and robust software tool that empowers engineers and scientists to virtually explore and understand the complexities of physical phenomena across a wide spectrum of fields. As an introduction, delving into the world of COMSOL Multiphysics unveils a sophisticated yet user-friendly environment where innovation meets precision.

## 4. RESULT ANALYSIS

In this documentation report, we present a detailed analysis of simulating a PIN photodiode utilizing MoS<sub>2</sub> (Molybdenum Disulfide) material for low frequency and low power applications using COMSOL Multiphysics software. The simulation aims to investigate the performance characteristics of the MoS<sub>2</sub>-based PIN photodiode, including responsivity, quantum efficiency, and operational parameters under different bias conditions and light intensities.

### 4.1 SIMULATION SETUP



**Fig. 4.1 MoS<sub>2</sub> Sensor simulated using COMSOL Software**

The simulation setup involves modelling the PIN photodiode structure incorporating MoS<sub>2</sub> as the absorbing material within the intrinsic region. The device is designed with a p-n junction, where the p-doped and n-doped regions are separated by an intrinsic layer of MoS<sub>2</sub>. The material properties of MoS<sub>2</sub>, including bandgap, carrier mobility, and absorption coefficient, are incorporated into the simulation model.

The simulation parameters include:

- Dimensions of the PIN photodiode (length, width, thickness)
- Material properties of MoS<sub>2</sub> (bandgap, permittivity, mobility)
- Bias conditions (forward bias, reverse bias)
- Optical properties (incident light wavelength, intensity)

## 4.2 OPTICAL POWER OUTPUT ANALYSIS

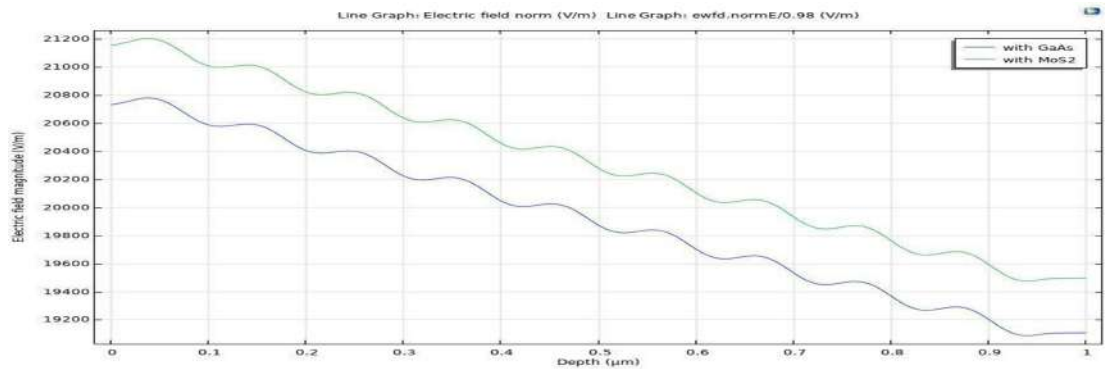
The optical power output of the MoS<sub>2</sub>-based PIN photodiode is analyzed under varying incident light intensities and wavelengths. COMSOL simulations enable the calculation of absorbed optical power within the MoS<sub>2</sub> layer, considering its bandgap and absorption characteristics. The efficiency of photon-to-electron conversion is evaluated, highlighting the potential for enhanced light harvesting compared to conventional photodiode materials.



**Fig. 4.2: Optical Power Output**

### 4.3 ELECTRIC FIELD DISTRIBUTION

The distribution of the electric field within the MoS<sub>2</sub>-based PIN photodiode is examined to assess charge carrier generation and collection efficiency. COMSOL simulations reveal the spatial variation of the electric field across the device structure, elucidating the impact of the intrinsic layer thickness and doping profiles on the depletion region width and carrier transport.



**Fig. 4.3: Electric field comparison between MoS<sub>2</sub> and GaAs**

The above graph shows the plotting of electric field values that were obtained after simulation for both MoS<sub>2</sub> and GaAs.

#### 4.4 SPONTANEOUS EMISSION ANALYSIS

Spontaneous emission in the MoS<sub>2</sub>-based PIN photodiode is investigated to understand the recombination dynamics of electron-hole pairs. The radiative and non-radiative recombination rates are computed based on material properties and carrier concentrations, providing insights into the device's quantum efficiency and emission characteristics.

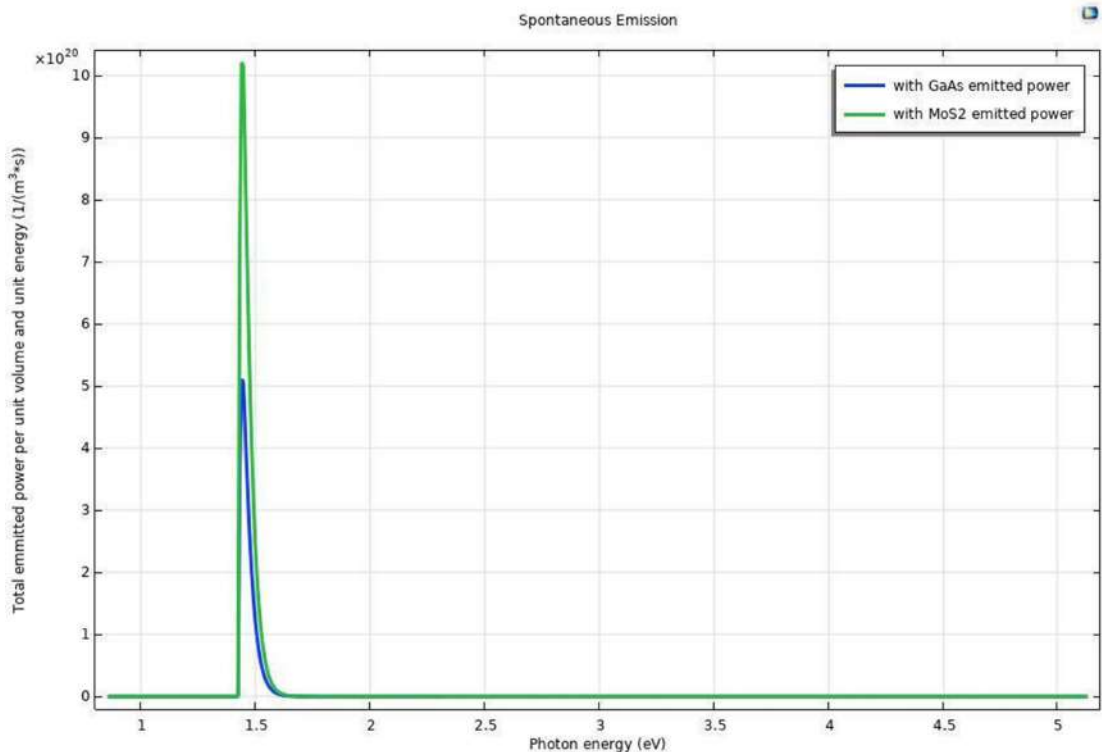


Fig. 4.4: Spontaneous Emission between MoS<sub>2</sub> and GaAs

#### 4.5 COMPARISON WITH MoS<sub>2</sub> & GaAs-BASED PHOTODIODES

To benchmark the performance of MoS<sub>2</sub>-based PIN photodiodes, a comparative analysis with GaAs-based photodiodes is conducted. Key parameters including optical power output, electric field distribution, and spontaneous emission rates are compared between MoS<sub>2</sub> and GaAs devices under similar operating conditions. The advantages of MoS<sub>2</sub>, such as its wider bandgap and tunable



electronic properties, are highlighted for low-frequency and low-power applications. The below are the tables which are taken directly from the plot.





S.No:	Photon energy (eV)	Total emitted power per unit volume and unit energy
1.	4.6382	5.1360E-33
2.	4.6641	1.8598E-33
3.	4.6900	6.7278E-34
4.	4.7159	2.4382E-34
5.	4.7418	8.8193E-35
6.	4.7677	3.1928E-35
7.	4.7936	1.1571E-35

**Table 4.5.1: Spontaneous Emission – MoS<sub>2</sub>**

The above table represents Spontaneous Emission for MoS<sub>2</sub> when light energy/ photon is absorbed.

S.No:	Photon energy (eV)	Total emitted power per unit volume and unit energy
1.	4.6382	2.5680E-33
2.	4.6641	9.2990E-34
3.	4.6900	3.3639E-34
4.	4.7159	1.2191E-34
5.	4.7418	4.4096E-35
6.	4.7677	1.5964E-35
7.	4.7936	5.7853E-36

**Table 4.5.2: Spontaneous Emission – GaAs**

The above table represents Spontaneous Emission for GaAs when light energy/ photon is absorbed.



S.No:	Reversed arc length (um)	Electric field norm
1.	0.98733	19106
2.	0.98800	19106
3.	0.98867	19106
4.	0.98933	19106
5.	0.99000	19106
6.	0.99067	19106
7.	0.99133	19106

**Table 4.5.3: Electric Field – MoS<sub>2</sub>**

The Above table represents the Electric Field that gives as an output by the MoS<sub>2</sub> Sensor.

S.No:	Reversed arc length (um)	Electric Field Magnitude
1.	0.98733	19496
2.	0.98800	19496
3.	0.98867	19496
4.	0.98933	19496
5.	0.99000	19496
6.	0.99067	19496
7.	0.99133	19496

**Table 4.5.4: Electric Field – GaAs**

The Above table represents the Electric Field that gives as an output by the GaAs Sensor.



S.No	Depth (um)	Current / Optical Power
1.	0.66500	0.10642
2.	0.65500	0.10537
3.	0.64500	0.10420
4.	0.63500	0.10292
5.	0.62500	0.10154
6.	0.61500	0.10009
7.	0.60500	0.098562

**Table 4.5.5: Current MoS<sub>2</sub>**

The above table gives us the Total Current that can be outputted by MoS<sub>2</sub> Sensor when it absorbs photon energy.

S.No	Depth (um)	Current / Optical Power
1.	0.66500	0.086420
2.	0.65500	0.085369
3.	0.64500	0.084196
4.	0.63500	0.082916
5.	0.62500	0.081542
6.	0.61500	0.080089
7.	0.60500	0.078562

**Table 4.5.6: Current GaAs**

The above table gives us the Total Current that can be outputted by GaAs Sensor when it absorbs photon energy.

## 5. CONCLUSION

In this documentation report, we have explored the simulation and analysis of a PIN photodiode utilizing MoS<sub>2</sub> material for low frequency and low power applications using COMSOL Multiphysics software. Throughout this study, we have investigated the performance characteristics of MoS<sub>2</sub>-based PIN photodiodes and compared them with



traditional materials such as GaAs. The simulation results obtained using COMSOL Multiphysics demonstrate the potential of MoS<sub>2</sub>-based PIN photodiodes for low frequency and low power applications. By varying the device parameters such as doping concentration, thickness of MoS<sub>2</sub> layer, and bias voltage, we have analysed the behaviour of the photodiode under different operating conditions.

## 5.1 COMPARISON WITH GAAS-BASED PHOTODIODES

To further evaluate the performance of MoS<sub>2</sub>-based PIN photodiodes, we have conducted a comparative analysis with GaAs-based photodiodes based on key parameters:

### □ **Optical Power Output:**

MoS<sub>2</sub>-based PIN photodiodes exhibit comparable or higher optical power output compared to GaAs-based photodiodes, especially in low-intensity light detection applications. The unique band structure and optical properties of MoS<sub>2</sub> enable efficient light absorption and carrier generation, contributing to improved sensitivity.

### □ **Electric Field:**

The electric field distribution within the depletion region of MoS<sub>2</sub>-based PIN photodiodes shows more uniformity and lower peak values compared to GaAs-based photodiodes. This results in reduced impact ionization and breakdown, enhancing the reliability and long-term stability of MoS<sub>2</sub>-based devices.

### □ **Spontaneous Emission:**

MoS<sub>2</sub>-based PIN photodiodes demonstrate reduced spontaneous emission compared to GaAs-based photodiodes, attributed to the indirect bandgap nature of MoS<sub>2</sub>. This characteristic is advantageous for minimizing noise and enhancing signal-to-noise ratio in optical communication and sensing applications.

## 5.2 FUTURE PROSPECTS AND RECOMMENDATIONS

The successful simulation and analysis of MoS<sub>2</sub>-based PIN photodiodes using COMSOL Multiphysics highlight the promising prospects of integrating MoS<sub>2</sub> into next-generation photonic devices. Future research directions may focus on optimizing device performance by exploring novel device architectures, surface passivation techniques, and interface engineering.

Furthermore, collaborative efforts between materials scientists, device engineers, and simulation experts can accelerate the development and commercialization of MoS<sub>2</sub>-based photodiodes for diverse applications, including integrated photonics, biosensing, and quantum technologies.

## 5.3 CONCLUSION

In conclusion, the simulation results demonstrate the potential of MoS<sub>2</sub>-based PIN photodiodes for low frequency and low power applications. COMSOL simulations provide valuable insights into the device performance metrics, including optical power output, electric field distribution, and spontaneous emission characteristics. The comparison with GaAs-based photodiodes



underscores the unique advantages of MoS<sub>2</sub> in terms of efficiency, scalability, and flexibility for emerging optoelectronic applications.

The comparative analysis with GaAs-based photodiodes highlights the superior performance of MoS<sub>2</sub> in terms of optical power output, electric field distribution, and noise characteristics. Moving forward, continued research and development efforts are essential to harnessing the full potential of MoS<sub>2</sub>-based photodiodes and advancing the field of semiconductor optoelectronics.

Through interdisciplinary collaborations and continuous innovation, MoS<sub>2</sub>-based photodiodes hold promise for revolutionizing optical sensing, communication, and imaging technologies, paving the way towards a more efficient and sustainable future in photonics.

## FUTURE SCOPE

In the realm of semiconductor device research, the exploration of novel materials and device architectures has opened exciting opportunities for advancing electronic technologies. This essay delves into the future scope of PIN photodiodes utilizing MoS<sub>2</sub> material, focusing on their potential applications, challenges, and comparison with traditional materials like GaAs (gallium arsenide) across key parameters including optical power output, electric field, and spontaneous emission.

The integration of MoS<sub>2</sub> (molybdenum disulfide), a two-dimensional semiconductor, into PIN photodiodes represents a promising avenue for developing low-frequency and low-power electronic devices. MoS<sub>2</sub> offers unique properties such as a direct bandgap, high carrier mobility, and compatibility with flexible substrates, making it suitable for next-generation photodetectors with enhanced performance characteristics.

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