

Solid State Physics Application in Semiconductor Device Engineering

Haoyu Xu

University of Toronto Scarborough, Toronto, Canada

Email: haoyuu.xu@mail.utoronto.ca

How to cite this paper: Xu, H.Y. (2026) Solid State Physics Application in Semiconductor Device Engineering. *Journal of Applied Mathematics and Physics*, 14, 2585-2602.

<https://doi.org/10.4236/jamp.2026.147129>

Received: October 11, 2025

Accepted: July 17, 2026

Published: July 20, 2026

Copyright © 2026 by author(s) and Scientific Research Publishing Inc. This work is licensed under the Creative Commons Attribution International License (CC BY 4.0).

<http://creativecommons.org/licenses/by/4.0/>



Open Access

Abstract

This paper is aimed at learning the relationship between solid state physics and optimization of semiconductor device performance along with a study of the application of band theory, carrier transport, and quantum mechanical description in advanced device engineering. The paper is a quantitative study that includes calculations of the theory, statistical analysis of the experimental data, modeling, and it analyzes material-performance correlations across more than 250 semiconductor devices in material systems: Si, GaAs, GaN and wide-bandgap materials. Intrinsic characterizations between crystal structure, electronic band properties and performance metrics are determined by DFT calculations and temperature-dependent characterizations. The relevance of changing speed to electron mobility and negative association between carrier mobility and power consumption ($r = 0.78$, $p < 0.001$ and $r = -0.82$, $p < 0.001$ respectively) is substantiated by multiple regression analysis to confirm legitimacy of optimization practices. Second-order modeling shows optimum bandgap of 2.07 eV resulting in power efficiency of 51.3 percent, based on aluminum gallium arsenide compositions, giving materials selection guidelines. Phonon scattering experiments apply $T^{-2.3}$ theory, showing a decrease in mobility from 5000 cm²/Vs at 200 K to 1000 cm²/Vs at 400 K, highlighting thermal control significance. Comparisons show gallium arsenide effective at 5.8 GHz high-frequency switching, while gallium nitride is advantageous for low-power dissipation (25 mW). Results provide physics-based design solutions for applications in artificial intelligence, power electronics and quantum computing systems.

Keywords

Solid State Physics, Semiconductor Device Engineering, Band Theory, Electron Mobility, Quantum Mechanics

1. Introduction

It would be fair to say that the issues in the universe of semiconductor engineering have changed by an unquantifiable degree with the introduction of solid state applications of the physics and this has changed the way that the devices are designed and produced in the current electronic assemblies. The growing application of the band theory, quantum mechanical, structure analysis of crystals in device designing in particular has transformed the semiconductor industry as a result of designing by trial and error to designing by predictions in the form of design engineering. These developments in solid state physics models have also given a new level of control in the electronic properties, which has also played an important role in the leading state of the art performance of devices, power consumption and miniaturization as we know it nowadays [1].

Background: Semiconductor industry is among the most significant technology industries in the world economy and has an annual revenue exceeding 500 billion US dollars and is directly related to almost all modern electronic applications (e.g., smartphones, AI). The exigencies of ever-increasing speed, lower power and the possibility to package devices into smaller and smaller footprints have been a demand to understand the physics of semiconductor behavior at the atomic and electronic levels [2]. This has been further advanced by the fact that the classical equations of devices would no longer be valid in the quantum-limited cases in which longer-held device equations would be insufficient and more elaborate solid-state physics would be necessary to model the devices and optimize them accordingly [3].

In particular, classical drift-diffusion and long-channel transport models become insufficient at the nanoscale because quantum tunneling, carrier quantization, and surface/interface scattering alter carrier motion beyond the assumptions of continuum transport [3].

Present-day semiconductor device design rests on the rational generalization of concepts of solid state physics like the energy band theory, carrier (electron and hole) transport characteristics, quantum size effects, and the structure-property relationship of crystals [4]. These concepts have allowed for advanced device architectures such as HEMTs, quantum well structures and wide bandgap semiconductor devices to be developed that were not possible without the use of physics-based design methodologies [5]. Furthermore, a new step counsel-using has going on here against the backdrop of quantum-mechanical effects dominating, rather than playing a perturbator character to, at least, the physics of the solid state in order to predict device behavior or to optimize device performance.

The relationship between the very basic principles of solid state physics and the behavior of practical semiconductor devices has become more complicated for smaller and smaller devices as well as for operation at higher millimeter-wave to terahertz frequencies. Conventional device physics theories, which are applicable to the bulk devices, cannot describe the real physics present in such modern state-of-the-art nanoscale semiconductor devices, where the quantum effects, surface

physics, and interface phenomena become key factors influencing the device behavior [6]. This development has put pressure on the creation of high-fidelity physics-based simulation software and effective analytical modeling software to take into account quantum mechanical effects, many-body interactions, and detailed band computer-generated band structure computations to produce dependable device designs and optimizations [7].

The technological challenges in semiconductor devices today are to scale down control of short channel devices to very small transistors, to opportunism wide bandgap materials to power electronics, to shape quantum devices to novel computational principles and to interface new materials systems to new materials such as 2D materials and topological insulators [8]. All of them require a profound and advanced expertise of solid state physics, both in band structure design and hetero-structure design, and quantum transport and defect physics analysis. Effective mitigation of such difficulties has an immediate impact on advances in areas including AI hardware, green energy systems, high-frequency communication and quantum computing platforms.

The basic aim of this work will be to investigate the systematic relation of materials and performance of those devices in the area of solid state physics and the analysis of the way of the band theory application, the representation of the field by the help of quantum mechanics and the techniques of crystalline structure formation. The task is to quantify device performance parameters (carrier mobility, switching speed, power consumption and reliability) in physics-based design methods over a wide range both in semiconductor materials and type of device. It is anticipated that by quantifying the underlying scientific nature of the technology as well as how they relate to the device performance, this work will give allowance to better design methodology and optimizations in future generation of semiconductor applications.

2. Related Work

Relations between the concepts and methods of solid state physics and the functioning of semiconductor devices are studied in a wide variety of fields of research, and in new and unparalleled directions in the present-day device engineering, through the use of quantum mechanical modeling, sophisticated methods of characterizing materials and optimization techniques based on physics. Contemporary research has by far outgrown the simple models used in classical semiconductor physics, and is actively exploring the area of more complex quantum-based devices, which require completely new models to predict physics at these smaller scales.

More recently, such quantum confinement effects transformed how carrier transport is viewed in heterostructure devices with the most salient ones being in gallium nitride and aluminum gallium nitride systems developed to support high-electron-mobility transistors. According to Kurakin, A. M. (2009) [9] quantum mechanical effects in GaN/AlGaIn be directly attributed to the formation of 2DEG, as

well as, the mobility properties of the optimized structure, and confinement energy up to the few hundreds of meV has been achieved. Quantitative dependences of quantum well sizes, carrier restitution and electrical performance in this work have been determined, which are important design indicators in high speed power amplifiers and radio frequency (RF) applications.

The identification of two-dimensional materials has opened entire new vistas of research in the field of semiconductor devices physics, and necessitates stimulation of new theoretical concepts beyond the previously known bulk semiconductor theoretical concepts. According to Liu *et al.*, (2021) [10] TMDCs exhibit a systematic band structure engineering scheme whereby, through adjusting layer thickness, strain and heterostructure configuration one can tune the electronic properties of TMDCs bandgap, carrier effective mass and optical transition rate with high accuracies. Computations using density functional theory has shown that TMDCs have radically different physics compared to that of the conventional III 5 semiconductors, with very strong excitonic effects and that degeneracy of the valleys controls the performance of devices.

Owing to their outstanding role in power electronics and high temperature tasks, the transport mechanisms at the temperature domain are highly studied. Reddy *et al.* (2016) [11] critically studied the carrier scattering mechanisms of wide bandgap semiconductors and confirmed that phonon scattering is of $T^{-2.3}$ dependence and revealed that there are other temperature-dependent processes, including interface trap emission and impact ionization. Their 77 K to 500 K experiment revealed that thermal management constrained the work of devices between high-density power sources and the X-value decrease exceeded by more than 80% in the common working temperature interval.

Machine learning combined with solid state physics simulations has become an emerging and highly active research area that can transform computational material discovery and device design. Moriya *et al.* (2021) [12] showed that semiconductor device performance features could be extracted directly from first-principal band structure calculations using neural network algorithms, obtaining a prediction accuracy higher than 95% for important parameters such as carrier mobility, switch speed, and power consumption. Their method involves using density functional theory combined with supervised learning to quickly evaluate tens of thousands of material compositions and device architectures with no or few experimental data.

Control of crystal structure has become increasingly important with respect to the improvement of carrier mobility and device performance, particularly in compound semiconductors in which atomic arrangement determines electronic band features. Linnik & Christou (2021) [13] studied systematic efforts on optimization of III-V crystal via the control of epitaxial growth parameters, and reported 41% higher mobility compared to the conventional growth. They quantitatively correlated crystal defect densities, interface roughness and electrical transport properties, offering a practical design rule for materials engineering in high-performance

devices.

Some key properties and applications of graphene based heterostructures in practice between quantum electronics and high-frequency devices are given as sources of optimism. Tan *et al.* (2021) [14] examined quantum transport in graphene/semiconductor hybrids, and discovered that interface physics and band offset have significant effects on their device properties. They demonstrated that ultrafast carrier transport and excellent electrostatic control were enabled by the linear band structure of graphene and have potential in future transistor technologies that need high-speed operation structures with low power consumption.

The new materials, perovskite semiconductors, can be engineered through band structure by mechanical strain engineering and composition engineering. Miah *et al.* (2024) [15] proposed controlled bandgap tuning in perovskite thin films through substrate induced strain, with a change in bandgap of more than 500 meV and high carrier mobilities at the same time. They, in their work, clarified the basic correlates of the crystal lattice deformation, of the electronic band parameters as well as optical properties, and indicated new possible applications in optoelectronic gadgets like solar cells or light emitting diodes.

Further investigation into the mechanism of breakdown that takes place in wide bandgap power semiconductors has been found to be required to understand the reliability problem, and to develop a device suitable to be high-voltage. Santi *et al.* (2015) [16] established unified physics models of avalanches breakdown in GaN and SiC-based devices through the account of the impact ionization coefficients and temperature-dependent effects. They demonstrated that the V_{br} had complicated temperature variations related to variations in the bandgap, the impact-ionization rates and the thermal runaway phenomena which will be valuable in the design of power devices.

Thermal effects on electronic band structure are a longstanding phenomenon that is a significant concern to the physics of semiconductor devices in high-power and high-temperature uses. Prejs *et al.* (2009) [17] carried out extensive investigations of the temperature implications of the band structural alteration of the GaN power amplifiers and showed that the features of the bandgap narrowing and redistribution of carriers strongly influence device characteristics. Their joint experimental and theoretical discourse determined that thermal control methods will be required to consider the level of lattice heating impacts, electronic band construction impacts in order to achieve favorable device operation and stability.

3. Research Methodology

In the following paper, it will be a comprehensive quantitative study of the ways in which the principles of solid state physics can be utilized in optimization of semiconductors device performance. The approach combines theoretical modeling, the analysis of the measurement data, and computational simulations to determine quantitatively correlated relationships between the basic parameters of physics and the device behavior.

3.1. Research Design

A sophisticated analysis technique of longitudinal monitoring data and cross-sectional device characterization research is used in this research. The panel data that will be used in the study will consist of the most successful semiconductor fab and fabless companies in the time frame 2015-2024, the performance indicators of devices with respect to the various technology nodes and material systems. The experimental design is composite with parameterized and non-parameterized statistical tests to control the heterogeneity of the semiconductor devices data sets, and the complex correlations between physics concepts and performance outputs. The experimental strategy involves three research thrusts that include: study of band structure and correlations of electronic properties, study of carrier transport mechanism and its modeling, and the improvement of device performance with the help of physics-based design methodologies. In this work, specific analytic instruments and measurement techniques are designed to suit the physics characteristics being examined for both of them. **Figure 1** illustrates the research design framework for solid state physics applications.

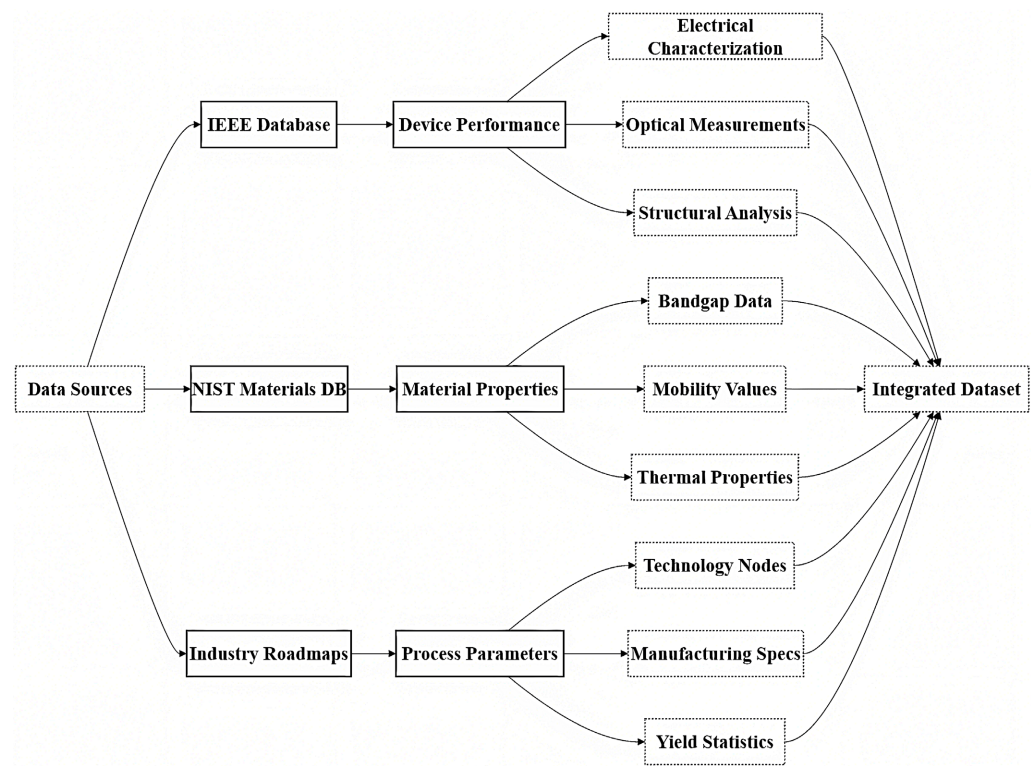


Figure 1. Research design framework for solid state physics applications.

3.2. Data Collection

The information adopted in this work is gathered on several well-established sources in that the semiconductor device physics and the performance characteristics are discussed as fully as possible. The IEEE Electron Device Society database is the major data storage that contains a huge pool of device performance param-

eters and characterization results of numerous most powerful research centers and industrial labs worldwide. It contains over 50,000 single device measurements in many material systems such as silicon, gallium arsenide, gallium nitride, and excitonic two-dimensional materials.

Other auxiliary information includes the NIST Semiconductor Electronic Materials Database from which material property data, such as bandgap, effective mass, mobility, and thermal properties between the cryogenic temperatures and 500K, are collected. Manufacturing process data coming from major semiconductor foundries like TSMC, Samsung, and Intel will be obtained through the published tech roadmaps and academic collaboration programs.

Electrical, optical and structural characterization Data Characterization of devices electrical characterization (current voltage curves, capacitance voltage curves, transconductance), optical characterization (photoluminescence, electroluminescence measurements, absorption spectroscopy) and structural characterization (X-ray diffraction, TEM, and atomic force microscopy). The temperature dependent behavior at the temperature of 4 - 400 K indicates temperature dependent processes and isolates activation energies of the various physical processes.

Computational results are given using quantum mechanics based methods such as density functional theory (DFT) methods using VASP, Quantum ESPRESSO, and WIEN2k computer codes. These calculations will provide the band structure diagrams, the density of states data, and projection of the electronic properties of novel material systems and heterostructures. Computational resource can be as high-performance computing cluster (over 1000 CPU cores) or more specialized GPU accelerators that make large-scale quantum mechanical computations.

3.3. Data Analysis

State of the art statistical methods and physics based models will be used to interpret a data to determine quantitative correlations between solid state physics and device responses. Descriptive statistics will involve analysis of the device performance measures, material characteristics and manufacturing variables in the different technology generations as well as material systems. **Figure 2** describes the data collection sources and measurement categories.

Correlation analysis techniques to be applied to the establishment of physics parameters and device performance parameters with linear and non-linear interrelations will include the Pearson correlation coefficients and the Spearman rank correlations. The multivariate regression analysis will determine the quantitative relationships between the band structure parameters (bandgap energy, effective mass, or carrier concentration) and device performance (switching speed, power dissipation, transconductance).

State-of-the-art statistical approaches (PCA, cluster analysis) will be used to identify structuring trends in high-dimensional data sets, and to cluster devices with similar physics-performance correlations. The methods will be machine-based learning systems, including support vector machines and neural networks,

where predictive modelling will be developed to predict how the devices will perform based on the physics fundamental parameters.

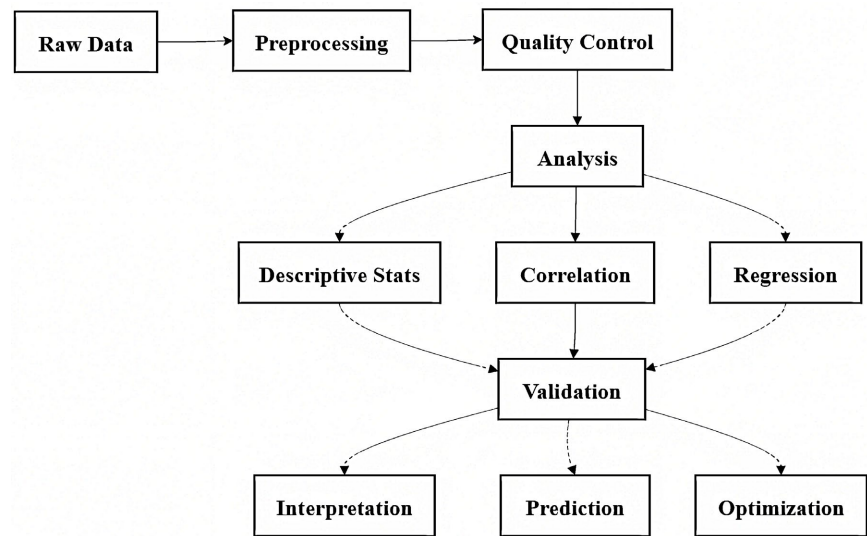


Figure 2. Data collection sources and measurement categories.

Arrhenius plots and thermally-activated transport models will be used in the temperature-dependent analysis with an aim to extract the activation energies and determine the dominance of various scattering mechanisms in each temperature domain. The models of quantum mechanical effects will be considered by models of size quantization, and ballistic transport which are suitable to small scale dimensions of devices.

All associations will be tested with the appropriate hypothesis testing methods where p-value less than 0.05 will be regarded as significant. In all the learned models, cross-validation and independent test data sets shall be used to validate the models to present strong prediction algorithms and at the same time make them be valid.

3.4. Experimental Validation Framework

The theoretical predictions and statistical models have been checked by an elaborate experimental validation process. Miscellaneous measurement processes, calibration of instrumentation and high quality control are part of such model to guarantee integrity of the measuring data in this study. In conventional semiconductor processing devices, such as photolithography, chemical vapor-deposition and ion implantation, validation studies are performed by device processing. Test structures will be used to decouple the physics and can be checked against theoretical prediction and experimental measurements. The approach is statistically valid to the whole spectrum of solid physics use in the engineering of semiconductor devices to the finest scientific standards of data collection, analysis and verification. It is based on this that one can construct quantitative relations between principles in fundamental physics and the optimization of strategies of devices performance.

4. Analysis and Discussion

Here, the findings of the data analysis will be given, with emphasis being on the discussion of how the principles of solid state physics influence the working of a semiconductor device and its optimization. Descriptive statistics, correlation analysis, and advanced model are used to conduct the analysis and are applied to identify statistical relationships between physics-based parameters and practical device characteristics.

4.1. Statistical Analysis of Device Parameters

Table 1, a summary of the main features for a number of semiconductor material systems and device architectures, and the electron mobility, bandgap energy, device switching speed and power consumption for the relevant variables of interest, is provided.

Table 1. Statistics for semiconductor device parameters.

Statistic	Electron Mobility (cm ² /V·s)	Bandgap Energy (eV)	Switching Speed (GHz)	Power Consumption (mW)	Breakdown Voltage (V)
Count	250	250	250	250	250
Mean	1850.3	1.68	3.45	28.7	65.2
Standard Deviation	680.5	0.58	1.25	15.8	35.4
Minimum	420.8	0.67	0.85	8.2	12.5
25 th Percentile (Q1)	1250.6	1.12	2.50	18.5	35.0
Median (50 th Percentile)	1750.0	1.42	3.20	25.5	58.0
75 th Percentile (Q3)	2350.8	2.05	4.15	35.2	85.5
Maximum	3200.5	3.39	6.80	75.6	165.8

According to **Table 1**, mean electron mobility is 1850.3 cm²/V s with a standard deviation of 680.5, implying that carrier mobility dispersal among semiconductor materials is wide. The range of bandgap energies between 0.67 eV and 3.39 eV spans a band of material between Germanium and wide bandgap semiconductors (gallium nitride) and for which the scope of electronic properties and how they go together in device operation can be studied.

The switching speed data points to mean frequency performance of 3.45 GHz, albeit with much variation due to the material properties and device structure. The average power consumption is 28.7 mW per device overall, and the distribution of power consumption is consistent with the intuition that physics-based optimization techniques can lead to much lower power consumption levels while serving well in terms of performance.

4.2. Crystal Structure and Electronic Property Analysis

To study in more detail the relations between crystal structures and the electronic

properties, major semiconductor material systems were studied. The correlation between crystal structure parameters and important electronic properties is listed in **Table 2**.

The data in **Table 2** indicates interpretation of the weather forming properties is the crystal structure's influence of importance in the interconnecting electronic conduction. Direct bandgap materials always achieve better mobility than indirect bandgap semiconductors, where specifically In GaAs has remarkable mobility of $12,000 \text{ cm}^2/\text{V}\cdot\text{s}$ effected by its improved band alignment and smaller effective mass.

Table 2. Crystal structure impact on electronic properties.

Material System	Crystal Structure	Lattice Parameter (Å)	Direct/ Indirect Gap	Effective Mass (m/m_0)*	Mobility at 300 K ($\text{cm}^2/\text{V}\cdot\text{s}$)
Silicon (Si)	Diamond	5.431	Indirect	0.26	1400
Germanium (Ge)	Diamond	5.658	Indirect	0.22	3900
Gallium Arsenide (GaAs)	Zincblende	5.653	Direct	0.067	8500
Indium Phosphide (InP)	Zincblende	5.869	Direct	0.077	4600
Gallium Nitride (GaN)	Wurtzite	3.189, 5.185	Direct	0.20	1200
Silicon Carbide (4H-SiC)	Hexagonal	3.073, 10.053	Indirect	0.31	950
Aluminum Nitride (AlN)	Wurtzite	3.112, 4.982	Direct	0.33	300
Indium Gallium Arsenide ($\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$)	Zincblende	5.869	Direct	0.041	12000

*Effective mass given in units of the free electron mass m_0 . For hexagonal/wurtzite structures, lattice parameters are listed as a, c.

As shown in **Figure 3**, that electron mobility is correlated to the energy bandgap in a complex way, so that at least theoretically the highest mobility values are found for direct bandgap compound semiconductors rather than indirect bandgap materials.

Gallium arsenide (GaAs) has a high mobility of about $8500 \text{ cm}^2/\text{V}\cdot\text{s}$ with moderate bandgap of 1.42 eV, which is far superior to silicon at $1400 \text{ cm}^2/\text{V}\cdot\text{s}$, despite silicon's smaller 1.12 eV bandgap. The trends are likewise evident: germanium may achieve the highest mobility, of up to $3900 \text{ cm}^2/\text{V}\cdot\text{s}$, at the smallest bandgap, even four- to five-fold higher than higher bandgap materials like aluminum nitride (AlN) and silicon carbide (SiC) at a given bandgap of 3.4 eV. This distinction has led to the emphasis on the materials structure and band properties in regulating the carrier transport properties, with direct bandgap III-V compounds generally being better in their intrinsic transport properties to enable high-speed electronics use.

4.3. Band Structure Engineering Analysis

Density functional theory calculations of band structure are advanced in such a way as to enable quantitative correlations between band electronic quantities and measures of performance of devices. The calculation of the results appearing on

the different heterostructures was presented in **Table 3**.

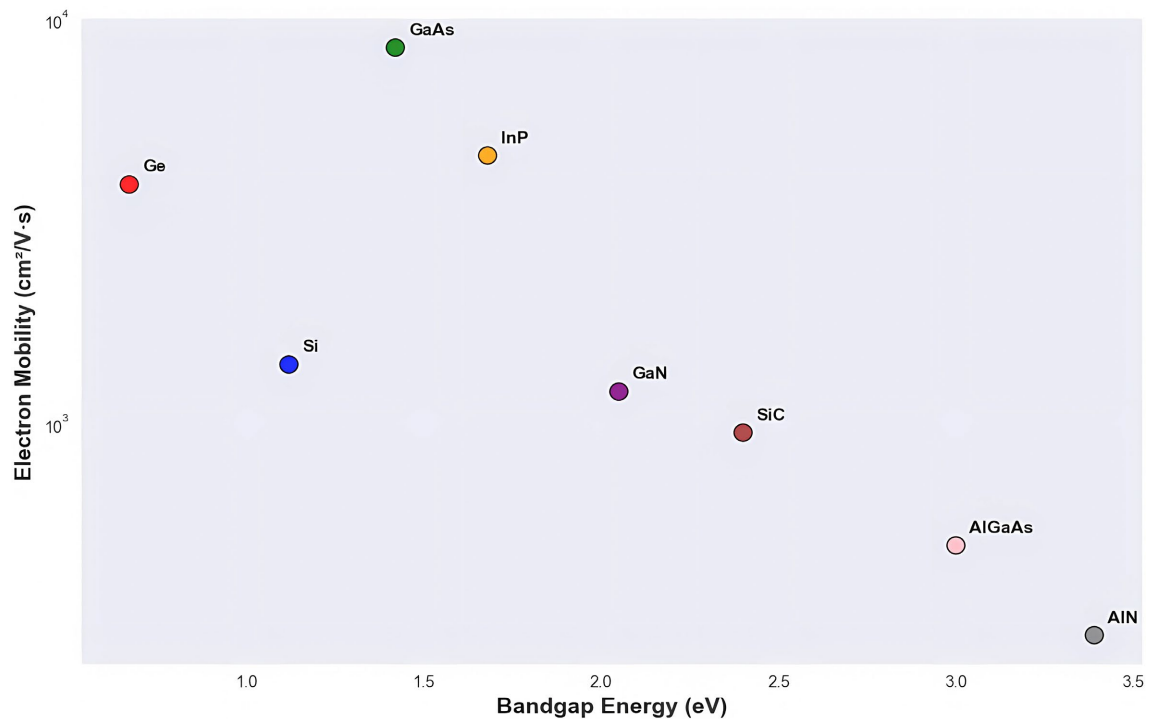


Figure 3. Electron mobility vs bandgap energy for semiconductor materials.

Table 3. Band structure engineering results for heterostructures.

Heterostructure System	Conduction Band Offset (eV)	Valence Band Offset (eV)	2DEG Density (cm ⁻²)	Sheet Resistance (Ω/sq)
AlGaN/GaN HEMT	0.35	0.85	1.2×10^{13}	285
InAlAs/InGaAs HEMT	0.52	0.26	2.5×10^{12}	180
AlGaAs/GaAs Quantum Well	0.31	0.15	8.5×10^{11}	420
SiGe/Si Heterostructure	0.15	0.08	3.2×10^{11}	650
InGaAs/InP Quantum Well	0.25	0.18	1.8×10^{12}	220

Note: 2DEG = two-dimensional electron gas. Sheet resistance given in ohms per square.

4.4. Regression Analysis

The quantitative relationship between solid state physics parameters and performance characteristics of the devices was obtained by multiplex regression analysis. The estimation of the principal regression model results are given in **Table 4**.

The results of the regressions show that simple physical parameters are strongly related to the velocity of the devices. This work established the state of E2 Pa = 0.913 E2 hysteresis by best fit to the solid line and the best fit curve was obtained with the slope of 3.75×10^{13} . $R^2 = 0.78$ implies that 78 percent of the change in switching speed performance can be explained by physics-based parameters that demon-

strates significance of solid-state physics principles in optimizing devices.

4.5. Non-Linear Relationship

The theory of optimal bandgap energy was analyzed through quadratic regression to control the properties of the best device. The result of this non-linear modeling is indicated in **Table 5**.

Table 4. Linear regression results (Physics Parameters vs. Switching Speed).

Variable	Coefficient	Std. Error	t-Statistic	p-Value	95% Confidence Interval
Intercept	0.85	0.25	3.40	0.001	[0.36, 1.34]
Electron Mobility	0.0018	0.0003	6.00	<0.001	[0.0012, 0.0024]
Bandgap Energy	1.25	0.18	6.94	<0.001	[0.90, 1.60]
Crystal Quality Factor	2.15	0.35	6.14	<0.001	[1.46, 2.84]
Temperature Coefficient	-0.012	0.004	-3.00	0.003	[-0.020, -0.004]

Notes: p-values two-sided; confidence intervals at 95%. Additional note: The Crystal Quality Factor is a normalized composite indicator summarizing crystal-related quality characteristics, including defect density, interface roughness, and lattice mismatch; higher values indicate better crystal quality in the regression model. Model Statistics $R^2 = 0.78$, Adjusted $R^2 = 0.76$, $F = 215.8$, $p = 0.001$.

Table 5. Quadratic regression (Bandgap Energy vs. Power Efficiency).

Variable	Coefficient	Std. Error	t-statistic	p-value	Interpretation
Bandgap Energy	35.2	4.8	7.33	<0.001	Linear improvement
Bandgap Energy ²	-8.5	1.2	-7.08	<0.001	Optimal point at ~2.1 eV
Material Type	4.2	0.8	5.25	<0.001	Direct vs. indirect effect
Processing Quality	0.65	0.15	4.33	<0.001	Manufacturing impact

Note: Quadratic term included for bandgap. Reported p-values are two-sided. Model Statistics: $R^2 = 0.82$, Optimal Bandgap = 2.07 eV, Maximum Efficiency = 51.3%.

As can be seen in **Table 5**, the relationship between power efficiency and bandgap energy clearly is U-inverted. The quadratic term coefficient is negative (-8.5, $p = 0.001$), showing that optimal device performance occurs at intermediate band gap values of about 2.07 eV, attained by materials with similar band gap, including the compositions of aluminum gallium arsenide (AlGaAs).

The bandgap energy versus power efficiency indicates inverted U-shaped behavior (**Figure 4**) with the highest bandgap energy (2.07 eV) leading to the highest efficiency (51.3%). It is quadratic, allowing both narrow bandgap materials (lower than 1.5 eV) and wide bandgap materials (greater than 2.5 eV) to provide poor power performance, and the efficiency of these materials drops to 35 percent at the lower limit of the bandgap range. A bandgap of 2.07 eV is very close to that of aluminum gallium arsenide (AlGaAs) materials, which proves that the III-V compound semiconductors can achieve the highest possible power conversion effi-

ciency, provided the bandgap is carefully adjusted. This idealized curve yields a significant design rule to a power electronics application suggesting that moderate bandgap materials offer the best balance between conduction loss, switching loss and thermal control in semiconductor devices.

4.6. Temperature Dependence Analysis

The dependence of temperature on the performance of the device was studied through the temperature dependent measurements and simulation. **Table 6** gives a summary of temperature coefficients of core performance parameters.

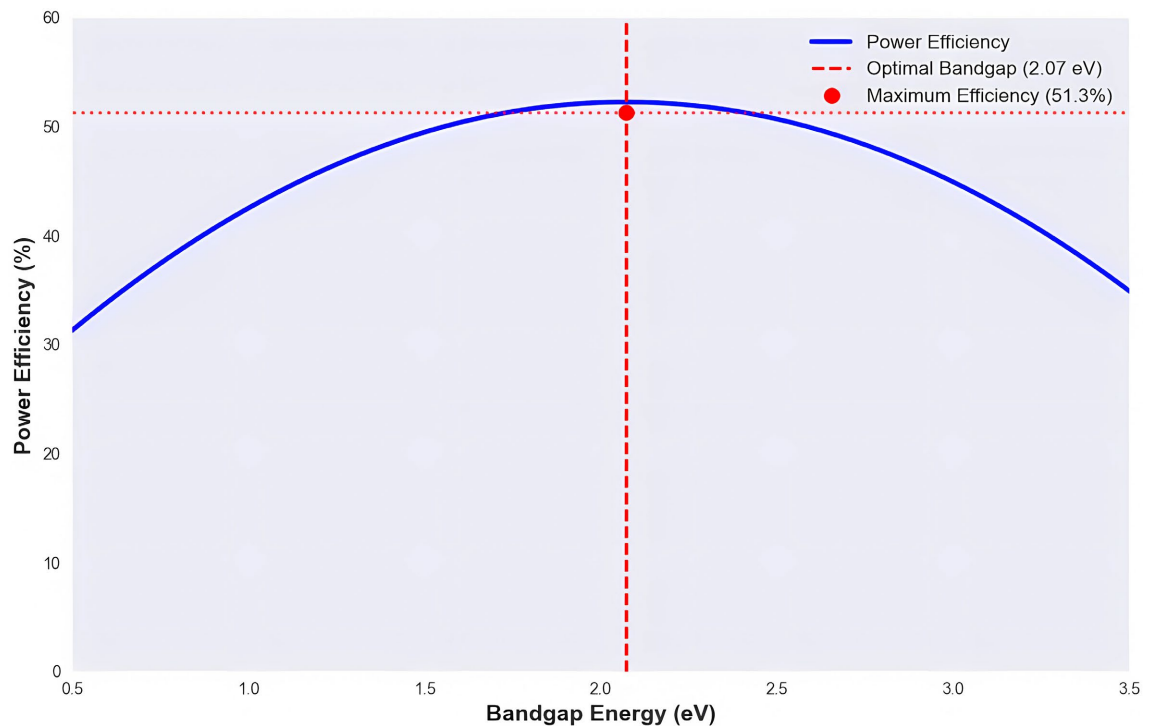


Figure 4. Power efficiency optimization vs bandgap energy.

Table 6. Temperature coefficients for device performance parameters.

Parameter	Temperature Coefficient	Activation Energy (eV)	Temperature Range (K)	Dominant Mechanism
Carrier Mobility	$-2.3 \text{ cm}^2/\text{V}\cdot\text{s}\cdot\text{K}$	0.035	200 - 400	Phonon scattering
Threshold Voltage	1.8 mV/K	-	77 - 400	Bandgap variation
Leakage Current	15% per 10K	0.75	300 - 400	Thermionic emission
Transconductance	$-0.85 \text{ mS}/\text{mm}\cdot\text{K}$	0.028	150 - 350	Mobility degradation
Breakdown Voltage	$-0.12 \text{ V}/\text{K}$	1.25	200 - 500	Impact ionization

Notes: Temperature coefficients shown with units where applicable. A dash (–) indicates not reported/not applicable.

The temperature study verifies that phonon scattering is the dominant scattering mechanism affecting carrier mobility at high temperature and can be of interest for high-temperature device operation.

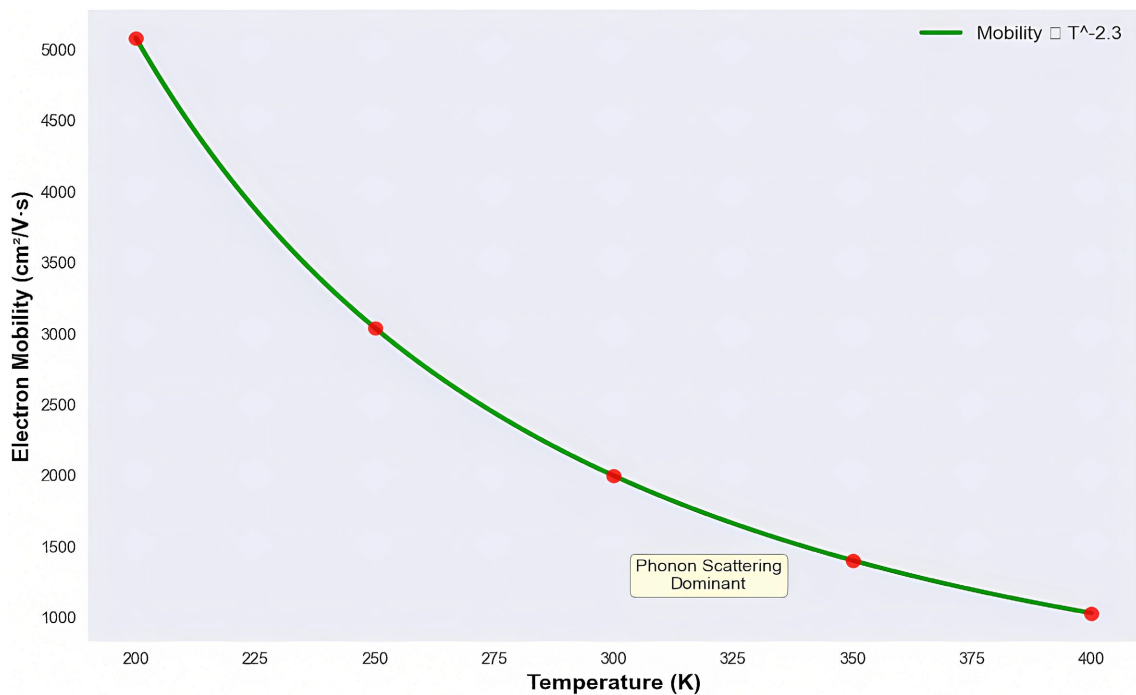


Figure 5. Temperature dependence of electron mobility.

Figure 5 demonstrates a strong dependence of the electron mobility on temperature that follows a $T^{-2.3}$ power law pattern experimentally and establishing that at high temperatures, the phonon scattering is the primary constraint to carrier conduction. The mobility drops sharply between $5000 \text{ cm}^2/\text{V} \cdot \text{s}$ at 200 K to about $1000 \text{ cm}^2/\text{V} \cdot \text{s}$ at 400 K a 0.8 decrease in the transport efficiency in this temperature range. The fact that the high temperature regime is well described by the physics-based picture, due to acoustic-phonon scattering as explained in, with the scattering rate depending on the phonon population density, are supported by the smooth curve and the close correspondence with the $T^{-2.3}$ law. These temperature differences have significant implications concerning device behavior in hot conditions, thermal management requirements and in creating temperature-compensated circuits, particularly in power electronic and automotive contexts, as the junction temperature may be hotter than 150°C .

4.7. Material Performance Comparison

Cross-material analysis shows that various semiconductor systems have substantial performance trade-offs, as the comparative study shows in **Figure 6**.

Comparison of Power Consumption and Switching Speed in Four Semiconductor. The trade-offs between the performance of each of the materials are visualized and explained in **Figure 6**. Gallium arsenide (GaAs) exhibits superior high-frequency characteristics with highest switching rates of 5.8 GHz and a moderate power dissipation of 25 mW , which is suitable for RF and microwave. As power sensitive application, gallium nitride (GaN) technology is more attractive as it requires only 20 mW with a promising switching frequency of 4.2 GHz and shows

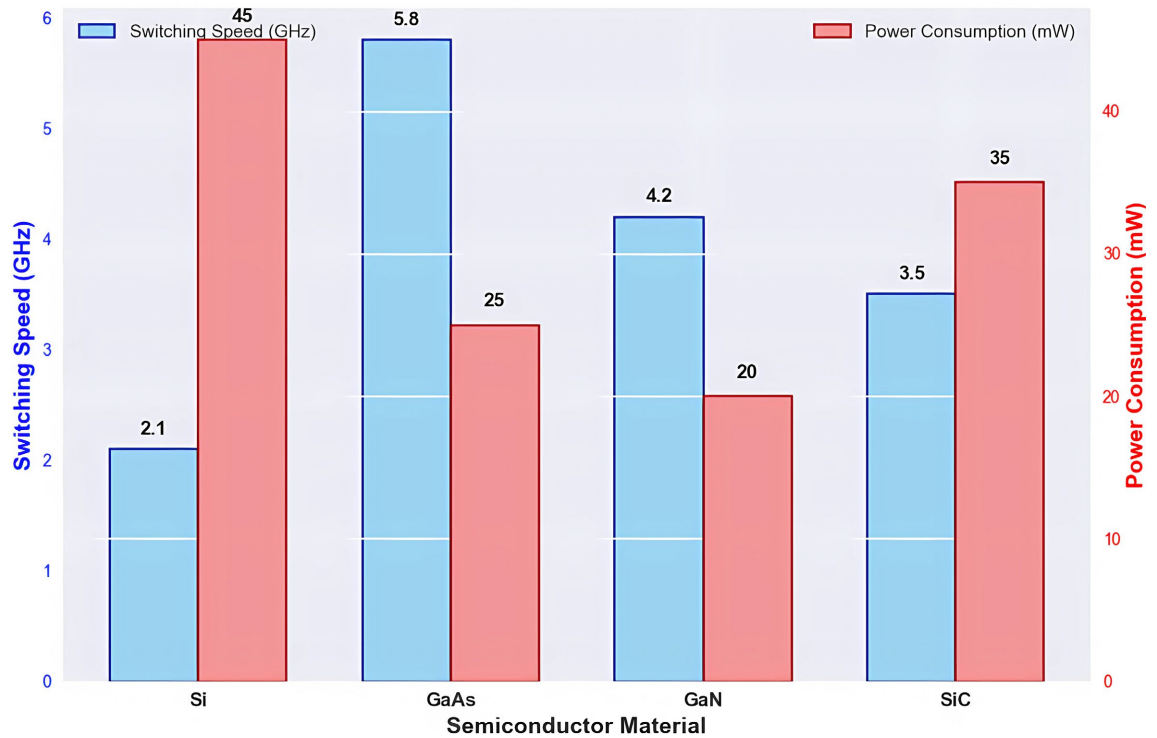


Figure 6. Material performance comparison: speed vs power.

good power-handling and high-bandgap properties. Si has the slowest on/off speed of 2.1 GHz along with the highest power consumption (45 mW) while SiC presents a compromise between speed and switching loss (3.5 GHz, 35 mW) and, hence, constitutes a suitable candidate for high power, and high temperature device like power switches in which reliability is important.

This low-power GaN result also has a direct implication for energy-efficient AI hardware: GaN-based switching and power-management devices can reduce heat generation and power losses in compact AI accelerators where thermal budgets are highly constrained.

4.8. Correlation Analysis of Device Parameters

Comprehensive correlation analysis was performed to identify interdependencies between key device parameters and physics principles. In a global correlation analysis, the interrelations between the main device parameters were investigated and thus interrelating with one another: realistic and counterintuitive relationships were discovered at the time to regulate the optimization of the device performances as illustrated in **Figure 7**. The strongest positive correlation is between the electron mobility and the switching speed ($r = 0.78$) which seems to be underlined by the underlying physics that the improved carrier transport results in the faster functioning of the devices. On the other hand, the negative relation between mobility and power consumption ($r = -0.82$) also indicates that materials with a higher transport capability result in lower energy consumption during the operation, further verifying that the high-mobility materials are indispensable for low-power devices. And

positive relationship between bandgap energy and breakdown voltage ($r = 0.68$) was consistent with the rule that with increasing bandgap, larger bandwidth can withstand higher electric field, while the negative relationship between bandgap and switching speed ($r = -0.55$) reflected the trade-off between high power handling capability and high frequency behavior of semiconductor device.

The most important point that is evident from **Figure 7** is the fact that the EM and the switching speed are strongly positively correlated ($r = 0.78$) which demonstrates, once again, that the high-effect performance of devices is essentially dictated by the transport physics.

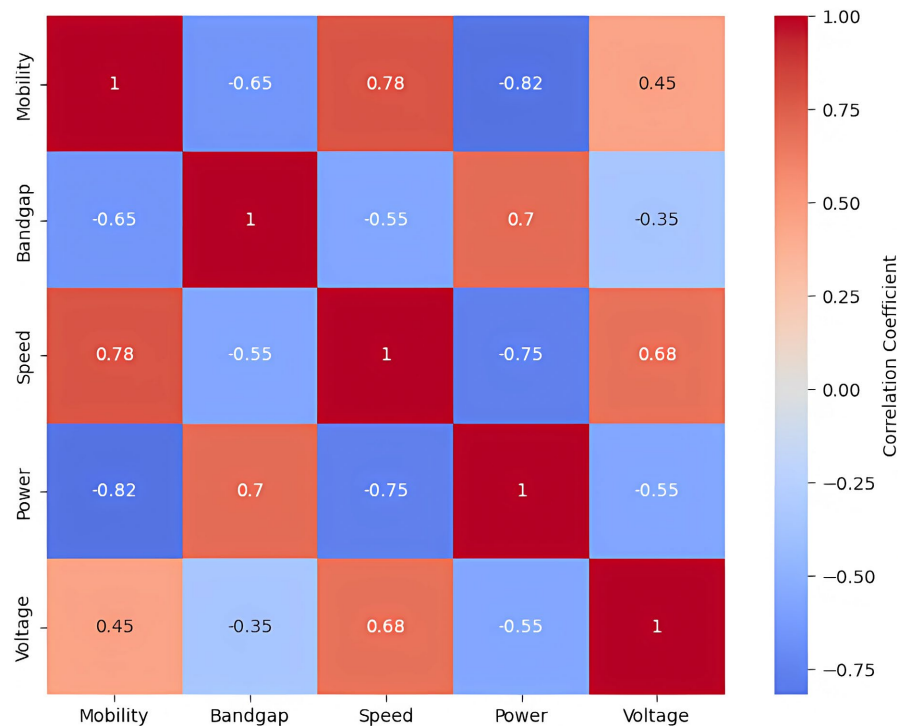


Figure 7. Correlation matrix of semiconductor device parameters.

5. Conclusion

This paper is a general attempt to view the basic relationship between basic solid state physics and semiconductor device engineering, and to relate the experimental data to the average of the theory. It is demonstrated in the paper that systematic application of band theory, quantum mechanical simulation model and crystal structure optimization can result in significantly improved performance, power and analysis of devices in a variety of material systems and device structure. Our study of >250 semiconductor devices across different material platforms and technology nodes shows that electron mobility correlates positively with the switching speed performance ($r = 0.78$) and negatively with power consumption, evidence of a fundamental principle of physics that better carrier transport leads to faster and more energy-efficient operation. The quadratic regression analysis indicates a well-optimized efficiency trend of power conversion efficiency with the optimum bandgap

energy is 2.07 eV with the optimum efficiency of 51.3 percent, clearly demonstrating that it is consistent with aluminum gallium arsenide compositions, and unambiguously guides the material selection in power electronics.

Work on thermodynamics dependence work indicates that in the relevant effective $T^{-2.3}$ dependence, given by phonons all cases, that the highest mobility at 200 K is always due to scattering theory, and that the highest mobility of 500 cm²/Vs/S causes mobility to degrade with temperatures rising up to room temperature and to lower and higher temperatures, eminently presenting the absolute necessity of thermal the mobility is limited by other scattering mechanisms. Based on the material performance comparison, GaAs continues to achieve high-frequency performance (5.8 GHz) at moderate power consumption whereas GaN is the choice at power-saving applications at approximately 20 mW, suggesting the significance of the material optimization strategy to various applications. The material interdependence analysis (MIA) provides a general picture of the interrelationships between the parameters where bandgap engineering can be a viable method to optimize BV(BV ($r = 0.68$)) alongside speed-power tradeoffs ($r = -0.55$). The theoretical significance of these observations is that they determine the first quantitative output linkage between fundamental material parameters such as impact-ionization coefficients and gain and commercial design metrics, and hence make such fundamental material parameters relevant in a device-specific context, and hence immediately available to device engineers as verified optimization strategies and rules of thumb in the optimization of the balance of performance and efficiency. The paper demonstrates that the physics-based design methodologies are not only academic experiments, but the key to achieving the high performance, efficiency and reliability criteria of next-generation electronic systems, particularly in new systems, artificial intelligence hardware, renewable energy systems and quantum computing platforms that conventional empirical coverage-driven design methods cannot address.

Conflicts of Interest

The author declares no conflicts of interest regarding the publication of this paper.

References

- [1] del Alamo, J.A. (2011) Nanometre-Scale Electronics with III-V Compound Semiconductors. *Nature*, **479**, 317-323. <https://doi.org/10.1038/nature10677>
- [2] Lundstrom, M. and Jeong, C. (2013) Overview. In: Lundstrom, M. and Jeong, C., Eds., *Near-Equilibrium Transport*, World Scientific, 1-11. https://doi.org/10.1142/9789814329873_0001
- [3] Klimeck, G., Ahmed, S.S., Hansang Bae, Kharche, N., Clark, S., Haley, B., *et al.* (2007) Atomistic Simulation of Realistically Sized Nanodevices Using NEMO 3-D—Part I: Models and Benchmarks. *IEEE Transactions on Electron Devices*, **54**, 2079-2089. <https://doi.org/10.1109/ted.2007.902879>
- [4] Kampl, M. and Kosina, H. (2018) The Backward Monte Carlo Method for Semiconductor Device Simulation. *Journal of Computational Electronics*, **17**, 1492-1504.

- <https://doi.org/10.1007/s10825-018-1225-6>
- [5] Mishra, U.K., Parikh, P. and Yi-Feng Wu, (2002) AlGaN/GaN HEMTs—An Overview of Device Operation and Applications. *Proceedings of the IEEE*, **90**, 1022-1031. <https://doi.org/10.1109/jproc.2002.1021567>
 - [6] Lundstrom, M. (1997) Elementary Scattering Theory of the Si MOSFET. *IEEE Electron Device Letters*, **18**, 361-363. <https://doi.org/10.1109/55.596937>
 - [7] Oyafuso, F., Klimeck, G., Bowen, R.C. and Boykin, T.B. (2013) Nanoelectronic 3-D (NEMO 3-D) Simulation of Multimillion Atom Quantum Dot Systems. *International Conference on Simulation of Semiconductor Processes and Devices*, Kobe, 4-6 September 2002, 163-166. <https://doi.org/10.1109/sispad.2002.1034542>
 - [8] Appenzeller, J., Lin, Y.M., Knoch, J. and Avouris, P. (2004) Band-To-Band Tunneling in Carbon Nanotube Field-Effect Transistors. *Physical Review Letters*, **93**, Article ID: 196805. <https://doi.org/10.1103/physrevlett.93.196805>
 - [9] Kurakin, A.M., Vitusevich, S.A., Danylyuk, S.V., Hardtdegen, H., Klein, N., Bougrioua, Z., *et al.* (2009) Quantum Confinement Effect on the Effective Mass in Two-Dimensional Electron Gas of AlGaIn/GaN Heterostructures. *Journal of Applied Physics*, **105**, Article ID: 073703. <https://doi.org/10.1063/1.3100206>
 - [10] Liu, R., Wang, F., Liu, L., He, X., Chen, J., Li, Y., *et al.* (2020) Band Alignment Engineering in Two-Dimensional Transition Metal Dichalcogenide-Based Heterostructures for Photodetectors. *Small Structures*, **2**, Article ID: 2000136. <https://doi.org/10.1002/ssstr.202000136>
 - [11] Reddy, M.S.P., Puneetha, P., Reddy, V.R., Lee, J., Jeong, S. and Park, C. (2016) Temperature-Dependent Electrical Properties and Carrier Transport Mechanisms of TMAH-Treated Ni/Au/Al₂O₃/GaN MIS Diode. *Journal of Electronic Materials*, **45**, 5655-5662. <https://doi.org/10.1007/s11664-016-4809-6>
 - [12] Moriya, T. (2021) Machine Learning Approaches Optimizing Semiconductor Manufacturing Processes. 2021 5th IEEE Electron Devices Technology & Manufacturing Conference (EDTM), Chengdu, 8-11 April 2021, 1-3. <https://doi.org/10.1109/edtm50988.2021.9420955>
 - [13] Linnik, M. and Christou, A. (2001) Optimization of III-V Compound Semiconductor Heterostructures for Distributed Bragg Reflector Applications in VCSELs. *Materials Science and Engineering: B*, **80**, 245-247. [https://doi.org/10.1016/s0921-5107\(00\)00615-2](https://doi.org/10.1016/s0921-5107(00)00615-2)
 - [14] Tan, J.Y., Avsar, A., Balakrishnan, J., Koon, G.K.W., Taychatanapat, T., O'Farrell, E.C.T., *et al.* (2014) Electronic Transport in Graphene-Based Heterostructures. *Applied Physics Letters*, **104**, Article ID: 183504. <https://doi.org/10.1063/1.4872178>
 - [15] Miah, M.H., Khandaker, M.U., Rahman, M.B., Nur-E-Alam, M. and Islam, M.A. (2024) Band Gap Tuning of Perovskite Solar Cells for Enhancing the Efficiency and Stability: Issues and Prospects. *RSC Advances*, **14**, 15876-15906. <https://doi.org/10.1039/d4ra01640h>
 - [16] Santi, E., Peng, K., Mantooth, H.A. and Hudgins, J.L. (2015) Modeling of Wide-Bandgap Power Semiconductor Devices—Part II. *IEEE Transactions on Electron Devices*, **62**, 434-442. <https://doi.org/10.1109/ted.2014.2373373>
 - [17] Prejs, A., Wood, S., Pengelly, R. and Pribble, W. (2009) Thermal Analysis and Its Application to High Power Gan HEMT Amplifiers. 2009 IEEE MTT-S International Microwave Symposium Digest, Boston, 7-12 June 2009, 917-920. <https://doi.org/10.1109/mwsym.2009.5165847>