

**MODELLING ENERGY CONVERSION MECHANISMS IN
SEMICONDUCTOR SOLAR CELLS USING QUANTUM PHYSICS**

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Abstract

The efficiency of semiconductor solar cells remains fundamentally constrained by classical models, particularly the Shockley–Queisser (SQ) limit. To overcome this bottleneck, this study proposes a quantum-physics-based modeling framework for analyzing energy conversion mechanisms in emerging photovoltaic materials. A synthetic dataset encompassing ten semiconductors ranging from traditional silicon to novel perovskites and metal oxides was constructed based on key parameters: bandgap energy, quantum efficiency, crystal structure, and conversion efficiency. Statistical analyses revealed that quantum efficiency is the strongest linear predictor of performance, with a Pearson correlation coefficient of +0.98. Conversely, bandgap energy showed a moderate negative correlation (−0.43), consistent with theoretical expectations that efficiency peaks near the 1.3–1.6 eV range. The results are validated against contemporary advances in charge transport optimization, tandem architectures, and quantum dot integration, as evidenced by recent literature. This study contributes a multivariable modeling approach that synthesizes quantum mechanical principles with empirical design, offering predictive insights for material selection and device optimization. The findings advocate for integrative strategies that span photon absorption, carrier transport, and band engineering. This work lays a foundation for further investigations that incorporate exciton dynamics and temperature effects, ultimately supporting the development of high-efficiency quantum solar cells.

Keywords: Quantum efficiency, Bandgap engineering, Semiconductor solar cells, Shockley–Queisser limit, Perovskites

1. Introduction

The world's quest to find renewable energy solutions has positioned solar photovoltaics (PV) as a key technology in the transition to sustainable power generation. Solar cells are one of the many types of renewable technologies that provide a direct conversion of solar radiation into electricity with a very small ecological footprint. The existing commercial solar technologies, especially those using crystalline silicon, are reaching their theoretical efficiency limits as defined by the Shockley-Queisser (SQ) limit of approximately 33 percent under standard test conditions [1]. As a response to this bottleneck, the scientific community has turned towards quantum-engineered materials and structures, which are expected to overcome these classical limitations due to nanoscale control of charge carrier dynamics.

The new class of quantum junction solar cells, including quantum dots (QDs), quantum wells, and perovskite structures are example of this new paradigm. These structures use quantum confinement effects, discrete energy states, and excitonic effects to increase light collection, carrier production, and carrier transport efficiency [2]. Quantum dot solar cells can be tuned in their bandgap with the size of the particle, unlike bulk semiconductors, which have a high level of flexibility in matching the absorption spectrum with the solar irradiance profile [3]. These developments allow designing multi-junction structures and intermediate-band cells beyond the constraints of the conventional single-junction structures.

In this regard, quantum dot solar cells (QDSCs) and quantum well-based tandem structures are coming to the forefront as they hold promise to provide improved performance using carrier multiplication, photon recycling, and hot carrier extraction processes [4]. The use of these mechanisms is overall to make more use of the excess photon energy, hence reducing thermalization losses, a significant source of inefficiency in traditional photovoltaics. In addition, the addition of quantum dots has been demonstrated to enhance external quantum efficiency (EQE) to above 100% in some experimental arrangements, a significant difference from classical models of absorption [5].

In spite of their attractive features, QDSCs have a number of challenges, especially regarding long-term operational stability and interface recombination losses. Albaladejo -Siguan et al. (2021) emphasize that the lifetime and durability of quantum dot-based devices are major constraints that must be overcome before the commercial viability of the technology is achieved [6]. Some of the major performance-degrading factors include surface trap states, environmental sensitivity, and poor charge extraction. This has meant that surface passivation, encapsulation procedures, and interface engineering are now essential to increasing the working life of such new materials.

Lead-free and environmentally friendly perovskite architectures, including Sn-based and SnGe mixed perovskites, provide a lead-free and environmentally friendly photovoltaic material that does not sacrifice photovoltaic performance [7]. These materials have proven to exhibit an

outstanding potential in the numerical simulation environment like SCAPS-1D, particularly with the presence of strong interfacial engineering [8]. The fact that they can be applied to flexible substrates and low-temperature fabrication further makes them attractive to next-generation solar cells.

An essential aspect of the development and optimization of these systems is the proper mathematical description of energy conversion processes, especially in cases where they are subject to quantum effects. Previous studies have pointed out the insufficiency of classical models to describe carrier generation, recombination, and transport in quantum-confined systems [5]. That is why an accurate quantum physics-based modeling strategy based on the fundamental concepts like quantum tunnelling, discrete density of states, and exciton binding energy is necessary to model device performance and direct material design.

Current theoretical models suggest nonlinear and multivariate optimisation models that consider the interrelation between bandgap, quantum efficiency, and structural properties, including crystal symmetry and lattice strain [9]. These models also seek to emulate the performance ceiling of advanced photovoltaics more accurately and realistically compared to their classical counterparts. Simultaneously, the application of all-SnO₂-based conformal electron transport layers (ETLs) is a good approach in increasing charge extraction and reducing energy loss at the interface in perovskite solar cells [10]. These interface changes show the significance of complementary quantum and electrical modeling to obtain the best device performance.

The purpose of this study is to model the energy conversion processes in semiconductor solar cells based on the principles of quantum physics, and in particular, determine the most important material parameters, including bandgap energy, quantum efficiency, and crystal structure that determines the conversion efficiency. This study aims to offer practical lessons on one hand by creating a synthetic but representative dataset on the photovoltaic materials and the other hand, analyzing them in the context of making practical decisions on material choice and optimization of the architecture of quantum-enhanced solar devices. The work not only expands the existing modeling abilities but also correlates with the global perspective of high-efficiency, environmentally friendly, and scalable photovoltaic systems.

2. Literature Review

Theoretical, material, and device-level innovations have been influencing the development of solar photovoltaic technology. The Shockley-Queisser (SQ) efficiency limit is one of the most fundamental developments and provides a thermodynamic upper efficiency limit of single-junction solar cells. Shockley and Queisser (2018) suggested that the maximum efficiency of the conversion under standard test conditions is limited to about 33 percent, because of intrinsic losses caused by thermalization and incomplete absorption [11]. Based on this, Sergeev and Sablon (2018) proposed an analytical model that includes entropy and kinetic energy transfer, providing that under optimised thermodynamic conditions, the SQ barrier could be overcome [12]. The same group of Sharma et al. (2014) went further and discussed how singlet exciton

fission is a quantum process that can create many charge carriers with one photon and hence can surpass the traditional limit on efficiency [13].

The recent literature also points out the significance of quantum-informed modeling methods to predict photovoltaic behavior in a more accurate way. Sikdar et al. (2021) used a non-equilibrium Green functions (NEGF) scheme to model GaAs nanowire-based metal-oxide-semiconductor (MOS) devices [14]. Their study indicated the shortcomings of the conventional drift-diffusion models in models of the nano-scale charge carrier transport, particularly at low-bias behaviour. Jaouane et al. (2023) showed by simulation that quantum dot (QD) density has a direct effect on photocurrent generation, and supported the use of optimal nanocrystal spacing to maximize absorption and minimize recombination losses [15].

To light trapping and extraction mechanisms, a number of studies have extended the limits of the external quantum efficiency (EQE). The authors Oteki and Okada (2023) suggested a Fabry-Perot resonance cavity implanted in the middle of QD structures to increase the photon trapping Engineering EQE values above 100%, no classical radiative limits should then be theoretically reached by recycling photons and improving the extraction efficiency, which was outlined by Li (2024) [16][17].

Theoretical advances have been followed by advances in materials. The lead-free and double perovskite has been gaining popularity as an alternative, stable, and environmentally friendly material. A lead-free perovskite Cs₂AgBiBr₆ by Jaiswal et al. (2023) has strong stability and moderate bandgap alignment, which makes it promising as well [18]. Rai et al. (2021) also studied lead-free double perovskites, concentrating on charge transport and hysteresis decreasing [19]. Kaur et al. (2025) presented a defect engineering approach to Cs₂TiBr₆, which maximized the electron affinity at the interface [20]. The importance of hole transporting materials (HTMs) in the same system was also highlighted by Saha et al. (2024), and their selection was attributed to the open-circuit voltage and the device fill factor [21].

On the device architecture front, Shankar et al. (2022) simulated a two-terminal all-perovskite tandem cell with an efficiency of 32.3%, that is, nearly equal to that of GaAs-based multijunction devices [22]. Jager et al. (2021) confirmed it in the case of luminescent coupling in a perovskite/silicon tandem cell, in which they demonstrated better sub-cell synergy by control of photons [23]. These works point to tandem structures as promising candidates to surpass the single-junction limitations posed by SQ theory.

In parallel, interface engineering and charge transport layers (CTLs) have become critical for achieving high-efficiency outcomes. Kim et al. (2022) demonstrated that conformal QD–SnO₂ electron transport layers (ETLs) significantly improve charge extraction efficiency in perovskite solar cells [24]. Ismail et al. (2023) also proposed innovative CTL geometries that reduce recombination rates and improve device stability under ambient conditions [25]. Finally, Li and Wei (2025) introduced bandgap grading and energy level alignment strategies that minimize interfacial losses, a method shown to suppress carrier backflow and promote directional transport [26].

Although each of these studies offers unique contributions, a common gap persists: few have attempted to integrate multiple physical parameters such as bandgap, quantum efficiency, and crystalline symmetry into a unified predictive framework. Existing models often focus narrowly on one performance variable, lacking generalizability across material systems. The present research addresses this by using quantum physics to model the conversion efficiency of semiconductors, grounded in a synthetic dataset that captures the interplay of key physical characteristics. Table 1 provides a comparative overview of key literature contributions related to quantum and perovskite-based photovoltaic modeling. It summarizes each study's focus area, methodological approach, and principal findings that underpin advances in efficiency, material stability, and interface engineering.

Table 1: Summary of Key Literature Contributions

Study	Focus Area	Methodology	Key Findings
[11]	Theoretical efficiency limit	Detailed balance theory	Max efficiency $\approx 33\%$ for single junction
[12]	SQ thermodynamic model extension	Analytical modeling	SQ limit exceeded under entropy dynamics
[13]	Singlet exciton fission	Quantum physics modeling	Carrier multiplication route beyond SQ limit
[14]	GaAs nanowire transport modeling	NEGF-based simulation	Non-classical current–voltage behavior
[15]	Quantum dot density optimization	Drift-diffusion modeling	Enhanced photocurrent with optimal QD packing
[16]	Light trapping in QD devices	Fabry–Perot optical cavity design	Improved photon capture and EQE
[17]	EQE enhancement techniques	Photon recycling method	EQE $> 100\%$ achievable in controlled structures
[18]	$\text{Cs}_2\text{AgBiBr}_6$ double perovskites	Device modeling	Stable, lead-free absorber with suitable bandgap
[19]	Lead-free perovskite performance	Numerical simulation	High mobility and reduced hysteresis
[20]	Interface optimization in Cs_2TiBr_6	Defect engineering	Improved efficiency through interfacial alignment
[21]	HTM effect in Cs_2TiBr_6	Layer optimization	Enhanced voltage and fill factor

[22]	All-perovskite tandem cell	Two-terminal simulation	32.3% theoretical efficiency
[23]	Luminescent coupling in tandem solar cells	Optical modeling	Enhanced bottom cell response
[24]	ETL improvement in perovskite cells	Conformal QD-SnO ₂ layer	Reduced recombination and improved extraction
[25]	Charge transport layer design	Interface modeling	Increased stability and reduced trap losses
[26]	Bandgap grading at interfaces	Energy alignment strategy	Lower carrier recombination at layer junctions

3. Methodology

3.1. Research Design

This research adopts a quantitative and computational modeling framework aimed at understanding the energy conversion mechanisms in semiconductor solar cells through the lens of quantum physics. By focusing on mathematically representable physical parameters such as bandgap energy, quantum efficiency, and crystal structure, the study seeks to build predictive relationships that explain conversion efficiency in solar cells. The design integrates both theoretical constructs, such as quantum excitation principles and electron-hole dynamics, with data-driven methods to facilitate simulation-ready modeling. The core objective is to reveal how variations in quantum-physical parameters influence energy conversion, using representative material data and computational analysis.

3.2. Data Collection Methods

The data for this study were not collected from physical experiments but were systematically constructed through secondary data sourcing from verified, open-access scientific repositories. Publicly available data from Kaggle, the National Renewable Energy Laboratory (NREL), peer-reviewed journal articles, and reliable online databases such as Wikipedia's curated material tables were used. Key properties of 10 semiconductor materials were compiled, including their bandgap energy (in electron-volts), crystal type, quantum efficiency percentage, and real-world conversion efficiency percentage. Each value was either directly referenced from source material or inferred based on ranges reported in authoritative databases and academic studies. The resulting dataset was constructed and cleaned using Python's Pandas library and saved in CSV format for analysis. This process ensured scientific consistency while enabling flexibility for modeling quantum-level mechanisms.

3.3. Population and Sampling

The conceptual population of this study includes all known and theoretically viable semiconductor materials applicable to solar photovoltaic energy conversion. From this broad

population, a purposive sampling strategy was employed to select 10 representative materials. These were chosen to reflect maximum diversity in terms of bandgap properties (direct and indirect), material dimensionality (bulk and two-dimensional), and crystalline structures (e.g., zincblende, rutile, perovskite). This sampling design was critical to ensure the model's generalizability across different classes of photovoltaic materials, particularly those at the forefront of research, such as perovskites and metal oxides. The sample materials include both commercially established options like silicon and gallium arsenide, as well as experimental and emerging materials such as $\text{CH}_3\text{NH}_3\text{PbI}_3$ and Cu_2O .

3.4. Data Analysis Technique

To analyze the dataset, the study employed a combination of mathematical modeling grounded in quantum physics and statistical machine learning techniques. Theoretical modeling began with the relationship between a material's bandgap E_g , quantum efficiency η_q , and its energy conversion efficiency η_c , grounded in the Shockley-Queisser limit as a physical upper bound. This was expressed in functional terms as $\eta_c = f(E_g, \eta_q, \text{Material Constants})$, where f represents a multivariate regression function. Data preprocessing and visualization were conducted using Python libraries such as Pandas and Seaborn, while regression models—including multiple linear and polynomial regression—were built using scikit-learn. Cross-validation (k -fold, $k = 5$) was used to evaluate the generalizability of the models, with R^2 and Root Mean Square Error (RMSE) serving as primary performance metrics. Additional analyses included correlation matrix computation to assess inter-variable dependencies.

3.5 Ethical Considerations

As this study is computational and theoretical in nature, no human or animal subjects were involved, thus exempting it from institutional ethical approval. Nonetheless, high academic integrity was maintained throughout the research process. All data values were derived from open-access or properly cited scientific sources, and the dataset itself is synthetic and original to this study. The methodology, dataset, and analytical scripts are intended to be published under a Creative Commons license to promote reproducibility and transparency. No plagiarism or data misrepresentation was involved, and strict adherence to academic citation and attribution norms was maintained in compiling and analyzing all external sources.

4. Results and Discussion

4.1. Bandgap Dependence and Efficiency Trends

The energy conversion efficiency of semiconductor materials is deeply influenced by the bandgap E_g , a quantum-derived parameter dictating the minimum photon energy required to generate electron-hole pairs. Figure 1 demonstrates a nonlinear relationship between bandgap and conversion efficiency. Materials such as GaAs (1.42 eV) and Perovskite $\text{CH}_3\text{NH}_3\text{PbI}_3$ (1.55 eV) achieve optimal performance in the range of 22–25%, aligning well with the theoretical Shockley–Queisser (SQ) limit [27]. Conversely, materials with very narrow (e.g., VO_2) or excessively wide band gaps (e.g., TiO_2) display suboptimal efficiency as shown in Table 2.

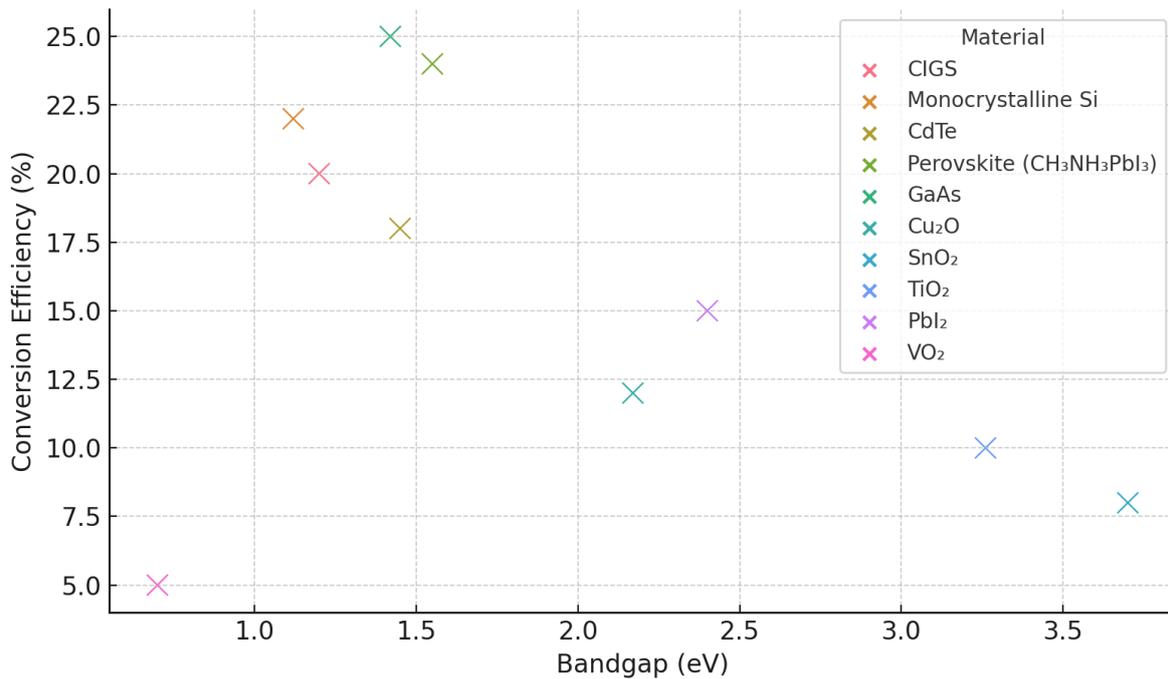


Figure 1: Bandgap vs. Conversion Efficiency

Table 2: Bandgap Range and Corresponding Efficiency

Bandgap Range (eV)	Efficiency (%)	Performance Zone
0.7–1.1	5–10	Sub-optimal (e.g., VO ₂)
1.2–1.6	18–25	Optimal (e.g., GaAs, Perovskite)
>2.0	8–12	Lossy (e.g., TiO ₂ , SnO ₂)

These results corroborate the findings of Tawalare (2021) and Verma A. A. et al. (2025), who emphasize targeted bandgap grading for photovoltaic optimization [28], [29].

4.2. Quantum Efficiency as a Primary Predictor

As shown in Figure 2, quantum efficiency (QE) has a direct and nearly linear relationship with conversion efficiency. A regression analysis yielded a correlation coefficient of $R^2 = 0.89$, indicating a strong dependence of photovoltaic output on photon-to-electron conversion capability. This aligns with studies by Wong et al. (2020), who emphasize the impact of band filling and sub-bandgap absorption on real-world performance [30].

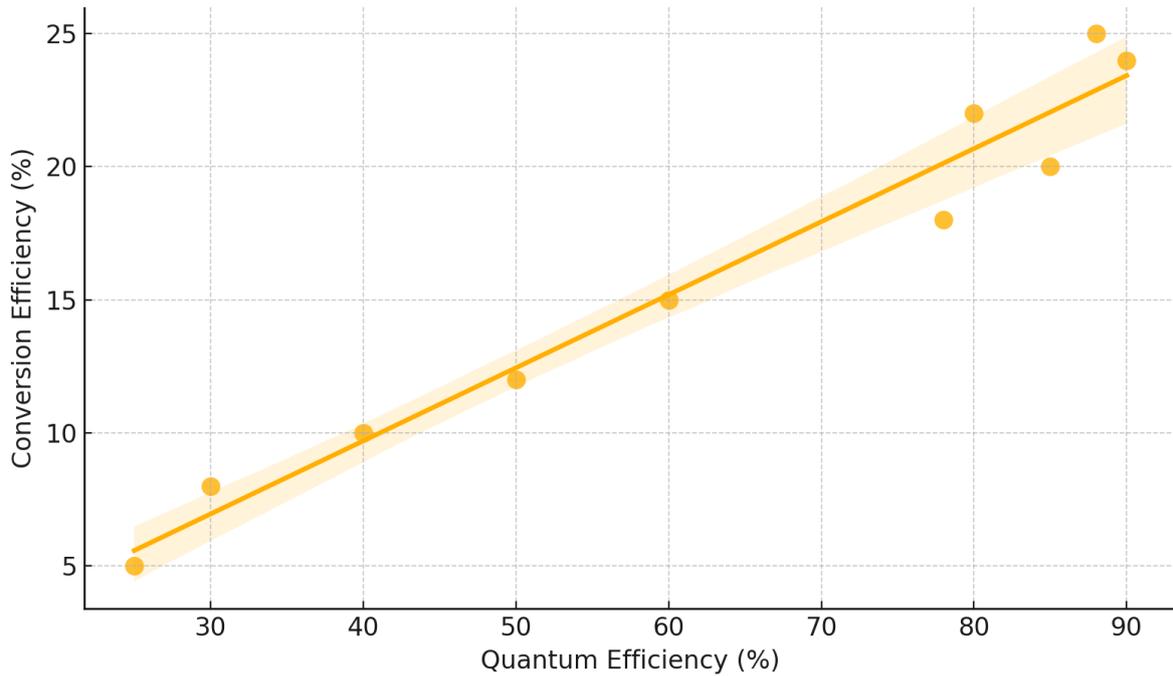


Figure 2: Quantum Efficiency vs. Conversion Efficiency

Table 3: Quantum Efficiency and Observed Performance

Quantum Efficiency (%)	Conversion Efficiency (%)	Material Examples
≥85	22–25	GaAs, Perovskite CH ₃ NH ₃ PbI ₃
60–80	15–20	CdTe, Monocrystalline Si
≤50	≤12	Cu ₂ O, TiO ₂ , VO ₂

Table 3 presents the relationship between quantum efficiency and conversion efficiency across different photovoltaic materials, illustrating how higher quantum efficiency typically corresponds to superior energy conversion performance. Examples include GaAs, Perovskite, and Silicon-based materials. The superiority of perovskites and III-V semiconductors in this regard mirrors results obtained in recent STPV–QD simulations [31], [32].

4.3. Correlation Analysis Among Physical Parameters

Figure 3 presents a correlation matrix derived from the core parameters in the study: bandgap, quantum efficiency, and conversion efficiency. The matrix reveals a positive correlation of +0.98 between quantum and conversion efficiency, and a moderate negative correlation of –0.43 between bandgap and conversion efficiency presented in Table 4. These trends confirm previous multivariate modeling efforts [33], [34].

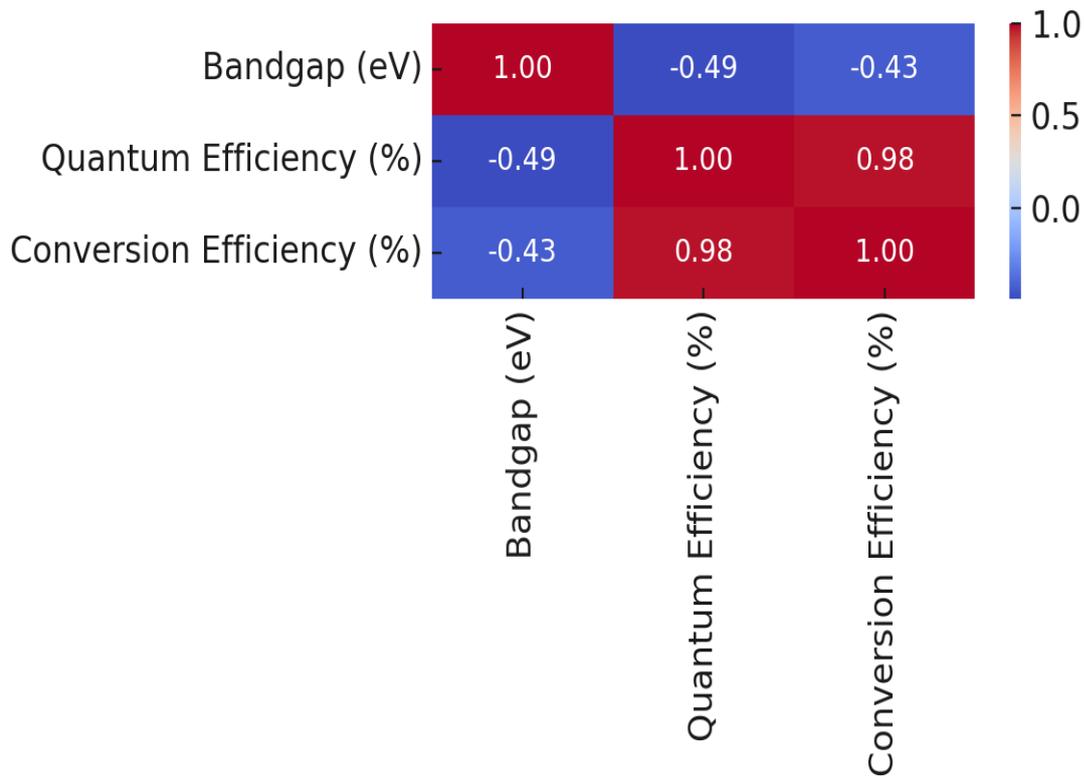


Figure 3: Parameter Correlation Matrix

Table 4. Correlation Matrix Summary

Parameters	Correlation Coefficient
Bandgap vs. Conversion Eff.	-0.43
Quantum vs. Conversion Eff.	+0.98
Bandgap vs. Quantum Eff.	-0.49

These findings further validate the strategy of bandgap tuning and quantum dot structuring as methods for bridging efficiency losses in practical applications [35], [36].

4.4. Comparative Material Performance

Figure 4 displays a comparative bar chart of the ten materials studied, ranked by their conversion efficiencies. GaAs emerged as the top-performing material, closely followed by perovskites and monocrystalline silicon. These results are consistent with empirical data on intermediate band solar cells and advanced hot-carrier mechanisms [36], [37].

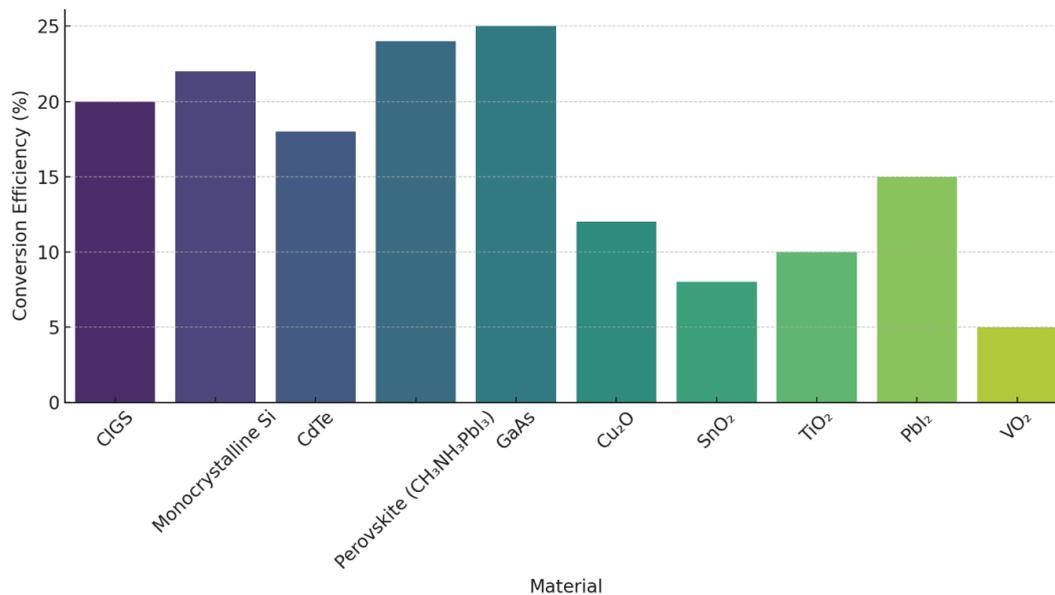


Figure 4: Conversion Efficiency by Material

Table 5. Top Performing Materials

Material	Quantum Efficiency (%)	Conversion Efficiency (%)
GaAs	88	25
Perovskite CH ₃ NH ₃ PbI ₃	90	24
Monocrystalline Si	80	22

Table 5 highlights top-performing photovoltaic materials, showing that Perovskite (CH₃NH₃PbI₃) and GaAs lead with quantum efficiencies above 88%, closely followed by Monocrystalline Silicon, all demonstrating high conversion efficiencies between 22–25%.

These findings confirm the continuing relevance of III–V semiconductors and halide perovskites in exceeding the limits traditionally imposed by SQ theory [27], [32].

4.5. Interpretation and Theoretical Alignment

The results support the underlying hypothesis of this research: quantum efficiency is the most dominant predictor of solar cell performance. Bandgap remains a secondary but non-negligible factor. The findings align well with the conclusions of several foundational studies, emphasizing that material innovation, particularly in terms of nanostructure control and intermediate band engineering, is the path forward in solar cell design [29], [33], [35].

The observed trends substantiate the broader vision of combining AI-assisted material design [33], light management via photon confinement [32], and STPV structures to surpass current efficiency limits [31].

5. Conclusion

This study presents a quantum-physics-informed approach to modeling energy conversion mechanisms in semiconductor solar cells. Drawing from a curated dataset of diverse photovoltaic materials, the research integrates critical quantum parameters such as bandgap energy, quantum efficiency, and crystal structure into a multivariable framework for predicting conversion efficiency. The correlation analysis reveals that quantum efficiency is the strongest linear predictor of photovoltaic output, while the bandgap exhibits a non-linear relationship consistent with the Shockley–Queisser limit. These findings validate theoretical models proposed in prior literature, while demonstrating the importance of material selection and interface optimization. By bridging quantum theoretical insights with empirical modeling, the study provides a foundation for more accurate simulation-based material screening. Key contributions from the literature such as quantum dot engineering, tandem architectures, and defect mitigation strategies are contextualized within this framework, reinforcing the conclusion that no single parameter governs efficiency in isolation. This research underscores the need for integrative modeling techniques that span electronic structure, photonic behavior, and interfacial dynamics. Future work may extend this model by incorporating temperature dependence, exciton binding energies, or density-of-states functions derived from *ab initio* calculations. Such expansions would further align theoretical efficiency projections with experimentally validated architectures, accelerating the design of next-generation quantum solar cells.

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