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Hot Carrier Dynarfmics: A Perspective on their Potential to Improve Next-Generation Photovoltaic Efficiency

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Abstract
The Shockley-Queisser limit, a theoretical efficiency limit of roughly 33%, is approaching for silicon-based solar cells, which presently control most of the photovoltaic (PV) market. The worldwide search for next-generation PV technologies with noticeably better performance has accelerated due to this limitation. The development of hot carrier solar cells (HCSCs), which seek to use photogenerated charge carriers before they lose surplus energy through thermalization, is one of the most promising strategies. Useful photon energy is quickly transformed into heat by this process. This energy loss mechanism substantially limits the efficiency of traditional solar cells.
HCSCs seek to overcome this limitation by incorporating materials with slow carrier cooling rates and energy-selective contacts that extract only carriers within specific energy ranges. These components enable higher photovoltage and improved energy conversion. This article explores the physics of hot carrier generation, thermal relaxation, and transport. It examines advanced materials such as lead halide perovskites, quantum dots, transition metal dichalcogenides, and III-V semiconductors that exhibit potential for hot carrier applications.
Recent experimental progress and theoretical models are discussed, along with the technological barriers that must be addressed—such as contact fabrication, thermal management, and material stability. With potential efficiencies exceeding 60%, HCSCs offer a transformative path toward ultra-high-efficiency photovoltaic systems.

Keywords: Hot Carrier Dynamics, Photovoltaics, Carrier Thermalization, Next-Generation Solar Cells, Efficiency Enhancement, Energy Selective Contacts

1. Introduction

As more environmentally friendly and sustainable energy sources gain popularity globally, solar energy has emerged as a crucial element of the revolution of renewable energy. It is an essential remedy for the twin problems of climate change and the depletion of fossil fuels because of its abundance, scalability, and low environmental effects (Maity et al., 2023). Over the past several decades, photovoltaic (PV) technologies—particularly single-junction silicon and thin-film solar cells—have grown in popularity and seen significant cost reductions (Ali et al., 2025). The Shockley-Queisser (SQ) limit, which limits the maximum theoretical conversion efficiency of single-junction cells to roughly 33%, indicates that these technologies are nearing the physical efficiency ceiling. The quick thermalization of photogenerated carriers is one of the main causes of this constraint. Absorption of photons with energy over the semiconductor band gap produces energetic electrons and holes, known as hot carriers. These hot carriers in traditional solar cells dissipate their surplus kinetic energy as heat in picoseconds after nearly instantaneously losing it through interactions with the lattice(Ghasemi et al., 2025). The rapid energy loss in modern PV systems is one of the main causes of inefficiency.

An inventive way to catch hot carriers before they thermalize involves using hot carrier solar cell technology (HCSCs) (Sum & Mathews, 2018). A significant amount of carrier energy is maintained using specially made energy-selective contacts, which could result in a notable increase in solar energy conversion. It is necessary to use materials with slow hot carrier cooling rates by nature and sophisticated device architectures that facilitate effective carrier collecting to realize this idea. The next generation of solar technologies could be revolutionized by HCSCs, which could provide power conversion efficiencies far over the SQ limit by resolving these problems (Masters, 2005). This study examines the material systems, design approaches, and theoretical underpinnings necessary to move hot carrier photovoltaics from theory to real-world application.

2. Objective of the Study

To analyze the physics, possibilities, and applications of hot carrier dynamics in solar photovoltaics and evaluate how they influence the development of next-generation, highly efficient PV technology.

3. Methodology

A qualitative and descriptive research methodology is used in this work to summarise the state of the art regarding hot carrier dynamics and how they might be used in next-generation photovoltaic (PV) systems. Because the research is based on secondary data sources, it guarantees a thorough and multidisciplinary comprehension of the topic (Twidell & Weir, 2006,).

Numerous credible, peer-reviewed scientific journals and internationally recognized research organizations provided the data reviewed for this study. High-impact journals that provide theoretical analyses and practical developments in hot carrier solar cell (HCSC) research, such as Nature Energy, Advanced Materials, Nano Letters, and Progress in Photovoltaics, are important sources. Energy-selective contact methods, device architecture, thermalization processes, and material behavior are all covered in these publications (Nozik et al., 2014).

This research integrates information from academic papers, technical studies, and innovation roadmaps published by prominent global organizations. The National Renewable Energy Laboratory (NREL) and the International Renewable Energy Agency (IRENA) have a great role in this context (International Renewable Energy Agency, 2016). These resources include important information on worldwide research trends, new developments in photovoltaic (PV) technology, and long-term forecasts for the use of solar energy (Ali et al., 2025). It also incorporates results from simulation studies and theoretical models that study microscopic carrier dynamics, phonon interactions, and energy loss mechanisms. Using sophisticated simulation tools makes predicting hot carrier behavior and device effectiveness under different design settings easier. Recent laboratory-scale experimental findings are examined when applicable, especially those about promising materials like two-dimensional materials like MoS_2 and WS_2, III-V compound semiconductors, lead halide perovskites, and colloidal quantum dots (Al-Waeli et al., 2019). The potential for supporting efficient hot carrier extraction and delayed carrier cooling is evaluated for these materials, and such qualitative methods are drawn to allow for a comprehensive and disciplinary understanding of hot carrier photovoltaics from various sources. It recognizes current research needs and opens up new avenues for creativity (Gong et al., 2024). This approach makes a thorough knowledge of hot carrier photovoltaics possible, which also highlights knowledge gaps and presents exciting prospects for further study and advancement and future research and development; this method allows for a full understanding of hot carrier photovoltaics. The qualitative synthesis seeks to bridge the gap between theoretical promise and real-world implementation by critically evaluating the field's chances and challenges.

4. Literature Review

More and more studies examine how hot carrier solar cells (HCSCs) could outperform traditional photovoltaic efficiency thresholds. This section examines ten significant contributions that cover hot carrier dynamics, experimental demonstrations, device engineering, material innovations, and theoretical underpinnings (Zhang et al., 2021).

4.1. Carrier Thermalization Losses in Conventional PV Systems

Green, (1981) identified the thermalization of photogenerated carriers as one of the principal energy loss mechanisms in single-junction solar cells, where more than 30% of incident solar energy is lost as heat. This process begins almost instantly after photon absorption, reducing the upper-efficiency limit to ~33%, known as the Shockley-Queisser limit.

4.2. Hot Carrier Dynamics and the Theoretical Basis for HCSCs

Nozik et al. (2014) first proposed the concept of hot carrier solar cells to bypass thermalization losses. Their work established that if carriers could be extracted before reaching thermal equilibrium, photovoltaic efficiency could exceed 60%. They emphasized the need for slow carrier cooling and energy-selective contacts to enable such extraction.

4.3. Hot Carrier Lifetimes in Emerging Materials

Yang et al. (2015) confirmed experimentally that methylammonium lead iodide ($CH_3NH_3PbI_3$) perovskites have extended hot carrier lifetimes, with durations surpassing 100 ps. Perovskites were identified as the top contenders for HCSCs because of this discovery, representing a substantial divergence from silicon's sub-picosecond lifetimes.

4.4. Energy Selective Contacts (ESCs)

Lee et al. (2017) modeled energy-selective contacts based on quantum tunneling and thermoelectric principles, demonstrating their theoretical ability to reduce entropy losses and maintain carrier energy during extraction. ESCs were shown to be essential for maintaining high photo voltages in HCSCs.

4.5. Graphene and Ultrafast Carrier Transport

Sun et al. (2008) explored carrier dynamics in graphene and found ultrafast carrier mobility and high thermal conductivity, which could be leveraged to manage heat in HCSCs while supporting fast transport. However, the lack of a band gap remains a limiting factor for photovoltaic applications.

4.6. Quantum Dot-Based Hot Carrier Effects

Konstantatos (2013) investigated colloidal quantum dots (QDs) and reported that quantum confinement in these nanostructures can significantly slow carrier cooling by reducing phonon scattering. They also emphasized the tunability of bandgaps in QDs, which could support spectral optimization in HCSC designs.

4.7. Transition Metal Dichalcogenides (TMDs)

Wang, (2013) examined hot carrier relaxation in monolayer MoS_2, a TMD with strong excitonic effects and slow thermalization behavior. They found that carrier cooling times can be extended to 50–200 ps under specific conditions, making TMDs attractive for ultrathin solar cell configurations.

4.8. Phonon Bottleneck in Nanostructures

Klimov (2012) examined how limited phonon states in quantum-confined systems cause a "phonon bottleneck" that slows energy dissipation. This process may improve hot carrier lifetimes, particularly in low-dimensional systems like superlattices and quantum wells.

4.9. Device-Level Simulations and Efficiency Projections

Polman et al. (2016) utilized detailed balance models to simulate HCSC performance under ideal conditions. They projected maximum efficiencies of up to 66%, provided hot carrier cooling and extraction are optimized. Their models also highlighted the need for tandem integration and spectral management.

4.10. Engineering and Material Difficulties

The scalable synthesis of hot carrier-supportive materials, heat control, and the fabrication of energy-selective connections are some of the practical difficulties in achieving HCSCs, as Nozik et al. (2014) outlined. He urged interdisciplinary initiatives that integrate materials science, device engineering, and photonics to further the area.

5. Hot Carriers Realizing hot carrier solar cells (HCSCs): It requires a thorough approach that includes developments in materials, device architecture, heat management strategies, and predictive modeling. These are the primary technological approaches being researched to increase solar efficiency by utilizing hot carrier effects (Kahmann & Loi, 2019).

5.1. Material Innovation

The choice of material is critical for slowing carrier cooling and sustaining hot carrier populations long enough for extraction. Emerging material systems include:

- **Lead Halide Perovskites (e.g., $CH_3NH_3PbI_3$):** These materials are distinguished by high absorption coefficients, low exciton binding energies, and inherent defect tolerance, all of which contribute to extended hot carrier lifetimes (often exceeding 100 picoseconds). Their favorable optoelectronic properties and ease of fabrication make them strong candidates for HCSCs (He & Galli, 2014).
- **Graphene and 2D Materials:** Graphene exhibits ultrafast carrier mobility (up to 200,000 $cm^2/V \cdot s$) and long carrier diffusion lengths, supporting efficient charge transport. Although it lacks a bandgap, its integration with other materials may enable hybrid architectures capable of efficient hot carrier extraction (Kotin et al., 2013).
- **III-V Semiconductors (e.g., GaAs, InGaP):** These materials offer high absorption coefficients and tunable bandgaps, allowing for efficient photon capture and potential for integration into tandem HCSC designs. Their strong excitonic behavior and nanostructuring capability enable control over phonon interactions and thermalization rates (Lee et al., 2022).

5.2. Thermalization Engineering

Engineering Thermalization:

The scientists create methods to slow carrier thermalization by managing phonon-mediated energy loss. There are two main methods which are:

- **Phonon Bottleneck Effect:** This is the process of making low-energy phonon modes that promote carrier cooling less accessible. **Phonon Bottleneck Effect:** This involves reducing the availability of low-energy phonon modes that facilitate carrier cooling. The discrete phonon spectrum slows down carrier-phonon interactions in quantum-confined systems like quantum dots or wells (Seebauer & Gorai, 2011).

- **Dielectric Confinement and Superlattices:** In heterostructures, the dielectric mismatch may impede phonon propagation. By preventing thermal energy transfer in dielectric confinement and phonon propagation, consecutive layer superlattices with separate acoustic characteristics could increase carrier longevity (Subramanian, 2001).

5.3. Architecture of Devices

The designs of next-generation HCSCs use several functional layers to maximize carrier extraction and reduce energy loss:

- **Energy-Selective Contacts (ESCs):** Dual ESCs for electrons and holes enable the selective extraction of carriers with energies above a defined threshold while blocking cooler carriers. This energy filtration maximizes voltage output (Limpert & Bremner, 2015).
- **Intermediate Energy Filters:** Layers with regulated band alignment can fine-tune carrier energy selection by eliminating entropy losses and enhancing device selectivity (Limpert & Bremner, 2015).
- Thermal management layers are incorporated to disperse surplus heat, stop material deterioration, and preserve structural integrity, especially under high-flux operating circumstances (Lee et al., 2022).

5.4. Modelling and Simulation

- A key factor in directing the design of HCSCs is computational tools. The following are important strategies:
- Density Functional Theory (DFT) and ab initio techniques are useful for forecasting potential materials' energy band topologies, electronic relaxation durations, and carrier-phonon interaction intensities (Maurer et al., 2019).
- TRPL (time-resolved photoluminescence) and ultrafast spectroscopy Data modeling: Using these methods, device simulations can be validated and calibrated using empirical insights into carrier lifetimes.
- Device-level Modelling: Programs like TCAD, Centaurus, and SCAPS model entire HCSC structures while fine-tuning variables like spectral response, contact resistance, and thermal gradients (Leventhal et al., 2006).

6. Challenges and Limitations

Despite promising progress, several critical barriers remain in the path toward the commercial viability of hot carrier solar cells:

- **Carrier Cooling:** The foremost challenge is achieving a sufficient hot carrier lifetime (~100 picoseconds or longer) for effective extraction (Sum & Mathews, 2018). Most materials exhibit cooling times that are too short for practical application.
- **ESC Fabrication:** Major technological challenges include energy-specific and low-resistance energy-selective contact design and fabrication. Most current ESC designs decrease (Goswami et al., 2000) The device's efficiency, adding large series resistance or lacking enough selectivity.
- **Thermal Management:** Excess energy not harvested as electrical output accumulates as heat, risking thermal degradation of sensitive materials. Efficient passive or active heat dissipation strategies are essential to maintain long-term stability.

- **Material Stability:** Promising materials like perovskites and certain quantum dots exhibit limited environmental and thermal stability. They degrade under exposure to light, oxygen, and heat, presenting reliability issues that must be addressed before large-scale deployment.
- **Scalability and Integration:** Many of the advanced materials and nanostructures discussed are not yet compatible with large-scale manufacturing processes. Integrating these materials into commercially viable, stable, and cost-effective devices remains a significant challenge.

7. Discussion and Analysis

Creating hot carrier solar cells (HCSCs) offers a path to efficiencies far above the Shockley-Queisser limit, marking a paradigm change in photovoltaic technology (Kahmann & Loi, 2019). The main innovation is the extraction of photogenerated carriers before their excess energy is lost to lattice vibrations, a process known as thermalization. This quick process is one of the main reasons why traditional solar cells lose energy.

7.1. Efficiency Potential and Theoretical Grounding

Conventional silicon-based photovoltaics typically convert only ~20–24% of incident solar energy into electricity under standard test conditions, with the theoretical limit capped at ~33%. On the other hand, theoretical models developed by Nozik (2001) indicate that, in the right circumstances, HCSCs might reach efficiencies of over 60–66%. These predictions capture a wider range of solar irradiance by using extra photon energy that would otherwise be lost as heat.

7.2. Role of Material Properties

A key component of this strategy is creating and incorporating materials with slow hot carrier cooling rates. Because of their extended hot carrier lifetimes (~100–200 ps), high absorption coefficients, and defect tolerance, perovskites like $CH_3NH_3PbI_3$ have become attractive options. Similarly, quantum dots and transition metal dichalcogenides (TMDs) such as MoS_2 exhibit slower carrier relaxation because of quantum confinement and excitonic effects. These substances allow hot carriers to survive longer, essential for their prompt extraction.

Excellent optical characteristics and compatibility with nanostructuring techniques that improve phonon scattering, which further slows thermalization, are other advantages of III-V semiconductors like GaAs and InGaP. Long-term stability, synthesis complexity, and cost issues still exist, nevertheless (Lee et al., 2022).

7.3. Designing Energy-Selective Interactions

Energy-selective contact (ESC) deployment is a major roadblock to HCSC realization. These connections must permit the passage of carriers with a limited energy range while obstructing lower-energy, thermalized carriers. In theory, ESCs can optimize voltage output while maintaining energy distribution. However, the present conductivity and energy resolution manufacturing methods are quite challenging (Subramanian, 2001). Many experimental prototypes' expected efficiency improvement is diminished due to high resistance or intensive energy filtering.

7.4: Structural and Heat Issues

Thermal energy management is intrinsically tied to the extraction of heat carriers. Inadequate carrier extraction produces excessive heat, which might deteriorate device stability and material qualities. Advanced thermal interface materials, passive heat dissipation layers, or radiative cooling systems are needed to manage this thermal accumulation. Furthermore, materials like perovskites have low stability in the presence of moisture, UV light, and high working temperatures despite being great for carrier dyna mics. The improvement of stability is still a top research focus.

7.4: Structural and Thermal Issues

Thermal energy management is intrinsically related to hot carrier extraction. Inadequate extraction of carriers leads to excessive heat production, which might deteriorate device stability and material qualities. It takes radiative cooling systems, passive heat dissipation layers, or sophisticated thermal interface materials to manage this thermal accumulation. Furthermore, materials like perovskites have poor stability in the presence of moisture, ultraviolet light, and high working temperatures despite being great for carrier dynamics. Enhancing stability continues to be a top research focus.

7.5. Device Architecture and Simulation

It supports Innovative HCSC architectures designed with dual ESCs, intermediate filtering layers, and graded bandgap structures to optimize carrier separation and energy conversion. Simulation techniques like ab initio approaches, DFT, and device-level simulators (like TCAD and SCAPS) are used to understand material behavior better, optimize band alignments, and project performance under various operating situations (Subramanian, 2001). These models are essential for directing experiments and identifying workable combinations of materials and contacts.

7.6. Integration and Scalability Considerations

The laboratory-scale results encourage the scaling of technologies to commercial production, presenting several obstacles. Nanofabrication techniques required for ESCs and quantum-confined materials are expensive and unsuitable for mass manufacturing. Furthermore, interfacing HCSC components with standard solar cell module needs and rethinking packaging with interconnection and encapsulation technologies are required to maintain performance while ensuring durability (Limpert & Bremner, 2015). Nonetheless, the potential for HCSCs to be integrated into multi-junction architectures or used in spectral splitting systems opens new possibilities. For example, placing a hot carrier layer with a conventional silicon cell could enhance spectral utilization and overall device output without requiring full substitution of existing technologies (Limpert & Bremner, 2015).

The analysis demonstrates that hot carrier solar cells hold transformative potential in the future of solar photovoltaics. Their theoretical efficiency far exceeds current technologies, and recent breakthroughs in material science, quantum engineering, and photonic design show promising pathways forward. However, multiple technical, economic, and engineering hurdles remain, particularly in energy-selective contact fabrication, heat management, and long-term material stability.

For transition, HCSCs from conceptual promise to commercial reality. Collaboration among materials scientists, device physicists, chemists, and engineers will be crucial to overcome existing barriers and develop scalable, stable, and efficient hot carrier photovoltaic systems. With sustained research and innovation, HCSCs could redefine the boundaries of solar energy harvesting in the 21st century (Limpert & Bremner, 2015).

8. Conclusion

Hot carrier dynamics showcase a peculiar and transformative opportunity in pursuing ultra-efficient solar photovoltaic (PV) technologies (Polman et al., 2016). As silicon-based single-junction solar cells near their theoretical efficiency limit of approximately 33%, the need for disruptive innovation becomes increasingly urgent (Augusto et al., 2020). Hot carrier solar cells (HCSCs) offer a novel and scientifically grounded approach to overcoming this barrier by extracting photogenerated carriers before they thermalize, thereby preserving their excess kinetic energy for electrical conversion (Lin et al., 2023).

This paper has critically examined the fundamental physics of hot carrier generation, thermalization, and extraction and evaluated the role of emerging materials—such as perovskites, quantum dots, graphene, transition metal dichalcogenides, and III-V semiconductors—in prolonging carrier lifetimes. Developing energy-selective contacts (ESCs) is equally important, as it serves as the cornerstone of any HCSC design, enabling the selective collection of high-energy carriers while minimizing entropy losses (Lin et al., 2023). Engineering challenges remain formidable. Carrier cooling must be sufficiently delayed (≥100 ps), ESCs require greater energy selectivity and lower resistance, and thermal management strategies must be incorporated to handle excess heat without compromising device integrity. Additionally, many promising materials lack the environmental stability or manufacturing scalability required for commercial deployment.

The theoretical models project that HCSCs could achieve efficiencies exceeding 60%. This experimental effort already demonstrates lifetimes and carrier dynamics that support this goal (Lin et al., 2023). Simulation tools and ab initio models are helping refine material selection and device architecture, bringing HCSC technology closer to feasibility.

Hot carrier dynamics provide a powerful framework for rethinking solar cell efficiency. It works beyond traditional limitations. While significant scientific and engineering advancements are still needed, the foundation has been laid for a new generation of photovoltaic systems that could redefine global solar energy potential (Limpert & Bremner, 2015). If the barriers discussed are successfully addressed, HCSCs could spearhead the next revolution in clean energy, making solar power more efficient, accessible, and impactful than ever before.

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