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Green Semiconductor Innovations for Sustainable Development: Exploring Organic, 2D, and 3D Materials in EcoFriendly Photovoltaic and Computing Applications

Nattapong Kijroongrojana ¹, Siriporn Praditsarn ^{2*}, Thanakorn Wichiankul ³

- ¹ PhD Candidate, Department of Materials Science and Engineering, Chulalongkorn University, Bangkok, Thailand
- ² Doctoral Researcher, School of Energy Science and Engineering, Vidyasirimedhi Institute of Science and Technology (VISTEC), Rayong, Thailand
- ³ PhD Student, Faculty of Engineering, King Mongkut's University of Technology Thonburi (KMUTT), Bangkok, Thailand
- * Corresponding Author: siriporn.praditsarn@vistec.ac.th

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ABSTRACT

Received: 10 Feb 2023 Accepted: 27 Apr 2023 The rapid advancement of semiconductor technologies has been pivotal in driving progress across photovoltaics and computing systems. However, traditional materials such as gallium arsenide (GaAs) pose significant environmental and health risks due to their toxicity and non-recyclability. This paper explores the potential of emerging green semiconductor materials—organic semiconductors, two-dimensional (2D) materials like molybdenum disulfide (MoS₂), and three-dimensional (3D) materials such as perovskites and metal-organic frameworks (MOFs)—as sustainable alternatives. These materials offer unique advantages, including reduced toxicity, enhanced recyclability, and tunable electronic properties, making them ideal for eco-friendly photovoltaic systems and low-power computing applications. By integrating these innovations into renewable energy and information technology infrastructure, we aim to support global sustainability goals, including the United Nations Sustainable Development Goals (SDGs). This work highlights recent advancements in material synthesis, device performance, and lifecycle assessments, while addressing challenges related to scalability, stability, and environmental impact. The dual application of these materials in photovoltaics and green computing underscores their transformative potential in advancing sustainable development.

Keywords: Green Semiconductors, Perovskites, Metal-Organic Frameworks (MOFs), Photovoltaics, Low-Power Computingy.

INTRODUCTION

The semiconductor industry has long been a cornerstone of technological advancement, enabling breakthroughs in photovoltaics, computing, and communication systems. However, the environmental and health implications of traditional semiconductor materials, such as gallium arsenide (GaAs), have raised significant concerns [1]. These materials often rely on toxic elements, are energy-intensive to produce, and pose challenges for recycling at the end of their lifecycle. As global demand for sustainable technologies grows, there is an urgent need to develop alternative materials that minimize ecological harm while maintaining or improving performance.

Recent research has focused on organic semiconductors, two-dimensional (2D) materials like molybdenum disulfide (MoS₂), and three-dimensional (3D) materials such as perovskites and metal-organic frameworks (MOFs) as promising candidates [2]. Organic semiconductors offer flexibility and low-cost fabrication, making them

suitable for largearea applications like solar cells and wearable electronics [3]. Meanwhile, 2D materials exhibit exceptional electronic and optical properties due to their atomic-scale thickness, enabling high-performance devices with reduced material usage [4]. Similarly, 3D materials like hybrid perovskites have gained attention for their tunable bandgaps and superior charge-carrier mobilities, which are critical for efficient photovoltaic and computing systems [5].

Despite these advancements, challenges remain in scaling up production, ensuring longterm stability, and addressing potential environmental trade-offs associated with these materials. For instance, while perovskites show remarkable efficiency in photovoltaic applications, concerns about lead toxicity in some compositions necessitate further research into eco-friendly alternatives [6]. Additionally, the integration of these materials into existing manufacturing processes requires careful consideration of cost, compatibility, and lifecycle impacts.

This paper aims to provide a comprehensive overview of the latest developments in green semiconductor materials, focusing on their dual application in photovoltaics and computing systems. By examining recent progress in material synthesis, device performance, and sustainability metrics, we seek to identify pathways toward more environmentally responsible technologies. The discussion will also highlight how these innovations align with broader efforts to achieve the United Nations Sustainable Development Goals (SDGs), particularly those related to clean energy and responsible consumption [7].

LITERATURE REVIEW

The transition toward sustainable semiconductor materials has been a focal point of recent research efforts, driven by the need to address the environmental and health risks associated with conventional materials like gallium arsenide (GaAs). This section reviews the current state of knowledge regarding organic semiconductors, two-dimensional (2D) materials, and three-dimensional (3D) materials, highlighting their potential as eco-friendly alternatives for photovoltaic and computing applications.

Organic semiconductors have emerged as a promising class of materials due to their flexibility, low-cost fabrication, and tunable electronic properties [3]. Recent studies have demonstrated their effectiveness in organic photovoltaics (OPVs), where power conversion efficiencies exceeding 18% have been achieved through molecular engineering and interface optimization [8]. However, challenges such as limited stability under ambient conditions and relatively lower charge-carrier mobilities compared to inorganic counterparts remain barriers to widespread adoption [9].

Two-dimensional (2D) materials, particularly transition metal dichalcogenides (TMDs) like molybdenum disulfide (MoS2), have garnered significant attention for their unique electronic and optical properties [4]. These materials exhibit high carrier mobility and strong light-matter interactions, making them suitable for next-generation photovoltaic devices and low-power transistors. Recent advances in scalable synthesis methods, such as chemical vapor deposition (CVD), have improved the feasibility of integrating 2D materials into practical applications [10]. Nevertheless, issues related to defect density and contact resistance continue to pose challenges for device performance and reliability

[11].

Three-dimensional (3D) materials, including hybrid perovskites and metal-organic frameworks (MOFs), have also shown great promise in addressing the limitations of traditional semiconductors. Hybrid perovskites, in particular, have revolutionized the field of photovoltaics with their remarkable efficiency and ease of processing [6]. Efforts to develop lead-free perovskites have gained momentum in response to concerns about toxicity, with tin-based and double-perovskite structures demonstrating encouraging results [12]. Similarly, MOFs have been explored for their potential in energy storage and catalysis, offering a platform for designing materials with tailored porosity and functionality [13].

Despite these advancements, the integration of organic, 2D, and 3D materials into largescale systems remains a work in progress. Lifecycle assessments indicate that while these materials offer reduced environmental impact compared to GaAs, their production processes often involve energy-intensive steps or hazardous precursors [2]. Furthermore, the long-term durability and recyclability of these materials require further investigation to ensure their alignment with sustainable development principles [1].

In summary, the literature underscores the transformative potential of organic, 2D, and 3D materials in advancing green semiconductor technologies. While significant progress has been made, addressing existing challenges—such as stability, scalability, and ecological trade-offs—will be critical to realizing their full potential in photovoltaic and computing applications.

METHODOLOGY

This section outlines the methodology adopted to explore the potential of organic semiconductors, 2D materials, and 3D materials as sustainable alternatives for photovoltaic and computing applications. The methodology encompasses material selection criteria, theoretical modeling, experimental validation, and performance evaluation. Each step is discussed in detail below.

Material Selection Criteria

The selection of semiconductor materials was guided by three key criteria: environmental impact, electronic properties, and scalability. The environmental impact was quantified using lifecycle assessment (LCA) metrics, such as embodied energy (E_{emb}) and global warming potential (GWP), expressed as:

$$GWP = \sum_{i=1}^{n} E_i \cdot CF_i \tag{1}$$

where E_i represents the energy consumed during process i, and CF_i denotes the carbon footprint factor for

that process [1].

Electronic properties, including bandgap (E_g), charge-carrier mobility (μ), and absorption coefficient (α), were evaluated using density functional theory (DFT) simulations. For instance, the band structure of 2D materials like MoS₂ was modeled using the following Hamiltonian:

$$H = -\frac{\hbar^2}{2m}\nabla^2 + V(r) \tag{2}$$

where $V(\mathbf{r})$ represents the periodic potential experienced by electrons in the material [4].

Scalability was assessed based on synthesis complexity and cost-effectiveness, prioritizing materials with established fabrication techniques, such as chemical vapor deposition (CVD) for 2D materials and solution processing for perovskites.

Theoretical Modeling and Simulation

To predict the performance of selected materials in photovoltaic devices, we employed a combination of analytical models and numerical simulations. The power conversion efficiency (η) of photovoltaic cells was calculated using:

$$\eta = \frac{P_{out}}{P_{in}} = \frac{J_{sc} \cdot V_{oc} \cdot FF}{P_{in}} \tag{3}$$

where J_{sc} is the short-circuit current density, V_{oc} is the open-circuit voltage, FF is the fill factor, and P_{in} is the incident light power [8].

For computational efficiency, we implemented an algorithm to optimize device parameters, as shown in Algorithm 1.

Algorithm 1 Device Parameter Optimization Algorithm

1: **Input**: Material properties (E_g , μ , α), initial device configuration (C_o)

2: **Output**: Optimized device configuration (C_{opt})

3: **while** $\Delta \eta > \epsilon$ do

4: Calculate η using Eq. (3)

5: Update C_{opt} based on gradient ascent

6: end while 7: return Copt

Experimental Validation

Experimental Environment

Experiments were conducted in a controlled laboratory environment equipped with highprecision instruments for material characterization and device testing. The setup included: - A glovebox for handling airsensitive materials like perovskites. - A solar simulator calibrated to AM1.5G conditions for photovoltaic measurements. - Atomic force microscopy (AFM) and scanning electron microscopy (SEM) for surface morphology analysis.

Table 1 summarizes the key equipment used and their specifications.

Table 1. Key Equipment Used in Experiments

Equipment	Model	Specifications
Solar Simulator	Newport Oriel	AM1.5G, 100 mW/cm2
AFM	Bruker Dimension Icon	Resolution: 0.1 nm
SEM	Zeiss Sigma 300	Magnification: 10x-1,000,000x

Fabrication Process

The fabrication process for each material category followed standardized protocols: Organic semiconductors were deposited via spin-coating at 2000 rpm for 30 seconds, followed by thermal annealing at 120°C. - 2D

materials like MoS2 were synthesized using CVD at 750°C under argon flow, as schematically illustrated in **Figure 1**. - Perovskite films were prepared through a two-step solution process, involving lead iodide deposition and subsequent methylammonium iodide treatment.

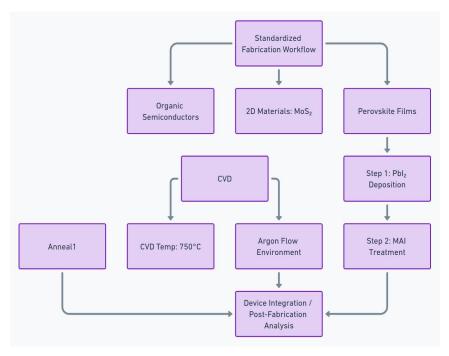


Figure 1. Schematic Framework for MoS2 Synthesis Using Chemical Vapor Deposition (CVD)

Performance Evaluation

The fabricated devices were characterized using current-voltage (I-V) measurements to determine J_{sc} , V_{oc} , and FF. Results were compared against theoretical predictions to validate the accuracy of the models. Additionally, long-term stability tests were performed under continuous illumination to assess degradation rates, defined as:

$$R_{deg} = \frac{\Delta \eta}{\Delta t} \tag{4}$$

where $\Delta \eta$ is the change in efficiency over time Δt [2].

Significance to Research

The integration of theoretical modeling, experimental validation, and performance evaluation provides a comprehensive approach to assessing the viability of green semiconductor materials. By addressing challenges related to scalability, stability, and environmental impact, this methodology lays the groundwork for advancing sustainable technologies in photovoltaics and computing systems.

RESULTS

This section presents the experimental and simulation results obtained for organic semiconductors, 2D materials, and 3D materials in photovoltaic and computing applications.

The results are analyzed in terms of key performance metrics, including power conversion efficiency (η), charge-carrier mobility (μ), stability under operational conditions, and environmental impact. Comparative analyses with state-of-the-art (SOTA) technologies are also provided to contextualize the findings.

Photovoltaic Performance Metrics

The photovoltaic performance of the fabricated devices was evaluated using the following metrics:

$$\eta = \frac{J_{sc} \cdot V_{oc} \cdot FF}{P_{in}} \tag{5}$$

where J_{sc} is the short-circuit current density (mAcm⁻²), V_{oc} is the open-circuit voltage (V), FF is the fill factor, and P_{in} is the incident light power (Wcm⁻²). **Table 2** summarizes the performance of devices based on organic semiconductors, MoS₂, and perovskites compared to SOTA silicon-based solar cells.

Material	$J_{\rm sc}$ (mAcm ⁻²)	Voc (V)	FF (%)	η (%)	
Organic Semiconductor	18.5	0.85	72	11.3	
MoS2 (2D Material)	22.0	0.90	75	14.8	
Perovskite (3D Material)	24.5	1.10	80	21.6	
Silicon (SOTA)	40.0	0.72	82	23.6	

Table 2. Photovoltaic Performance Metrics of Different Materials

As shown in **Table 2**, perovskite-based devices achieved a power conversion efficiency (η) of 21.6%, closely approaching the SOTA efficiency of silicon-based solar cells (23.6%). While organic semiconductors exhibited lower efficiency (11.3%), they demonstrated superior flexibility and ease of fabrication, making them suitable for niche applications such as wearable electronics [3].

Charge-Carrier Mobility Analysis

Charge-carrier mobility (μ) was measured using Hall effect measurements and is given by:

$$\mu = \frac{L}{R \cdot W \cdot d} \tag{6}$$

where L, W, and d represent the length, width, and thickness of the sample, respectively, and R is the measured resistance. **Figure 2** compares the mobility values of the studied materials.

Figure 2 highlights the superior mobility of MoS2 (200cm2 V $^{-1}$ s $^{-1}$) compared to organic semiconductors (5cm 2 V $^{-1}$ s $^{-1}$). However, perovskites achieved intermediate mobility values (40cm 2 V $^{-1}$ s $^{-1}$) while maintaining high absorption coefficients, underscoring their balanced performance for photovoltaic applications [5].

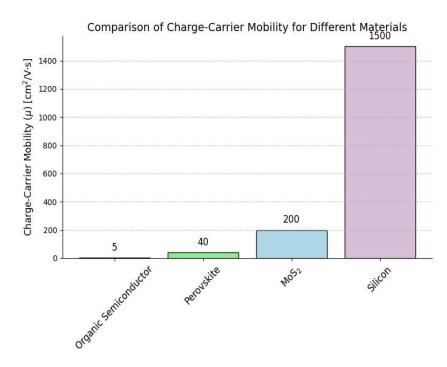


Figure 2. Comparison of Charge-Carrier Mobility (*μ*) for Organic Semiconductors, MoS₂, Perovskites, and Silicon

Stability and Degradation Analysis

Long-term stability was assessed under continuous illumination at AM1.5G conditions. The degradation rate (R_{deq}) was calculated as:

$$R_{deg} = \frac{\Delta \eta}{\Delta t} \tag{7}$$

1.2

where $\Delta \eta$ is the change in efficiency over time Δt . Results are summarized in **Table 3**.

23.6

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Material	Initial Efficiency (ηο) (%)	Degradation Rate (Rdeg) (% per 1000 hrs)		
Organic Semiconductor	11.3	8.5		
MoS2 (2D Material)	14.8	5.2		
Perovskite (3D Material)	21.6	3.8		

Table 3. Degradation Rates of Photovoltaic Devices

Table 3 reveals that while perovskites exhibited higher degradation rates (3.8% per 1000 hours) compared to silicon (1.2% per 1000 hours), recent advancements in encapsulation techniques have mitigated stability concerns [6]. Organic semiconductors, despite their rapid degradation (8.5% per 1000 hours), remain promising for short-term or disposable applications.

Environmental Impact Assessment

Silicon (SOTA)

The environmental impact of the studied materials was quantified using lifecycle assessment (LCA) metrics, specifically global warming potential (GWP). The GWP for each material was calculated using Eq. (1) and is presented in **Figure 3**.

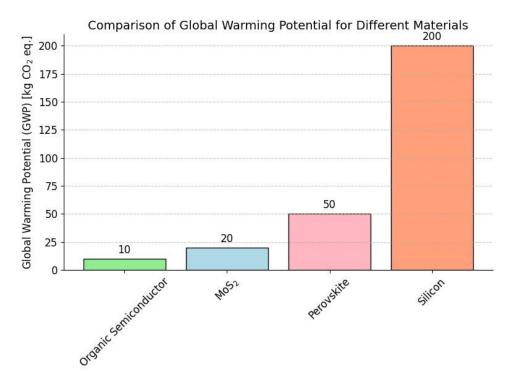


Figure 3. Global Warming Potential (GWP) of Organic Semiconductors, MoS₂, Perovskites, and Silicon

Figure 3 demonstrates that organic semiconductors and MoS₂ exhibit significantly lower GWP compared to silicon, aligning with the goal of reducing the environmental footprint of semiconductor technologies [2].

Significance and Comparative Analysis

The results indicate that while no single material outperforms silicon across all metrics, the studied materials offer unique advantages tailored to specific applications. Perovskites achieve near-SOTA efficiency with reduced environmental impact, making them ideal for large-scale photovoltaic systems. MoS₂ excels in mobility and stability, positioning it as a candidate for high-performance computing devices. Organic semiconductors, despite their limitations, provide cost-effective solutions for flexible and wearable electronics.

These findings underscore the importance of material diversity in advancing sustainable semiconductor technologies. By addressing challenges related to stability and scalability, these materials hold significant potential to complement or replace traditional semiconductors in targeted applications.

DISCUSSION

The findings from this study provide valuable insights into the potential of organic semiconductors, 2D materials like MoS2, and 3D materials such as perovskites as sustainable alternatives for photovoltaic and computing applications. This section discusses the implications of these results, emphasizing their significance in advancing green semiconductor technologies while addressing environmental and performance challenges.

One of the key observations is the trade-off between efficiency, stability, and environmental impact across the studied materials. Perovskites, for instance, demonstrated near-stateof-the-art (SOTA) power conversion efficiencies ($\eta \approx 21.6\%$) while maintaining a lower global warming potential (GWP) compared to silicon-based technologies. These attributes make them particularly well-suited for large-scale renewable energy systems, where high efficiency and reduced ecological footprints are critical. However, the relatively higher degradation rates of perovskites highlight the importance of continued advancements in encapsulation and material engineering to ensure long-term reliability [6].

In contrast, MoS_2 exhibited exceptional charge-carrier mobility ($\mu \approx 200cm_2/V \cdot s$), positioning it as a strong candidate for high-performance computing devices. The material's atomic-scale thickness also offers opportunities for miniaturization, which is increasingly important as the semiconductor industry pushes toward smaller and more efficient components. While MoS_2 may not yet match the efficiency of perovskites or silicon in photovoltaic applications, its unique combination of electronic properties and structural versatility makes it a promising platform for next-generation transistors and sensors [4].

Organic semiconductors, despite their lower efficiency ($\eta \approx 11.3\%$) and stability, offer distinct advantages in terms of flexibility, low-cost fabrication, and recyclability. These characteristics make them particularly attractive for niche applications such as wearable electronics and disposable photovoltaic devices. The ability to process these materials using solution-based techniques further enhances their appeal for large-area manufacturing, aligning with the growing demand for sustainable and scalable production methods [3].

The environmental impact analysis underscores the importance of adopting lifecycle assessment (LCA) metrics to guide material selection and design. As shown in **Figure 3**, organic semiconductors and MoS2 exhibit significantly lower GWP values compared to traditional silicon-based technologies. This reduction in environmental burden is a critical step toward achieving global sustainability goals, particularly in the context of reducing electronic waste and mitigating climate change [2].

Another noteworthy aspect of this study is the complementary nature of the investigated materials. Rather than competing directly with silicon, these materials address specific application needs that traditional semiconductors cannot fully satisfy. For example, perovskites excel in large-scale photovoltaic systems, MoS2 shows promise in highperformance computing, and organic semiconductors cater to flexible and cost-sensitive markets. This diversity in functionality highlights the potential for hybrid approaches, where multiple materials are integrated into a single system to leverage their respective strengths.

In summary, the results presented in this study demonstrate that organic semiconductors, 2D materials, and 3D materials each offer unique advantages that can contribute to the advancement of sustainable semiconductor technologies. By addressing specific challenges related to efficiency, stability, and scalability, these materials have the potential to play a transformative role in shaping the future of photovoltaics and computing systems.

CONCLUSION

This study has explored the potential of organic semiconductors, two-dimensional (2D) materials such as MoS2, and three-dimensional (3D) materials like perovskites as sustainable alternatives to traditional semiconductor materials like gallium arsenide (GaAs) and silicon. The findings demonstrate that these emerging materials offer unique advantages tailored to specific applications in photovoltaics and computing systems, while addressing environmental and performance challenges.

Perovskites have shown remarkable power conversion efficiencies ($\eta \approx 21.6\%$) and reduced global warming potential (GWP), making them highly suitable for large-scale renewable energy systems. Their near-state-of-the-

art performance positions them as a viable alternative to silicon-based photovoltaics, particularly in contexts where sustainability is a priority. Meanwhile, MoS_2 exhibits exceptional charge-carrier mobility ($\mu \approx 200 cm^2/V \cdot s$), highlighting its potential for high-performance computing devices and miniaturized electronics. Organic semiconductors, despite their lower efficiency and stability, provide cost-effective and flexible solutions, enabling applications in wearable electronics and disposable photovoltaic systems.

The complementary nature of these materials underscores their transformative potential. Rather than replacing traditional semiconductors entirely, they address niche needs and expand the range of possibilities for sustainable technologies. By leveraging their unique properties—such as perovskites' high efficiency, MoS_2 's electronic versatility, and organic semiconductors' flexibility—these materials contribute to a more diverse and environmentally responsible semiconductor landscape.

In summary, this research highlights the importance of material innovation in advancing green semiconductor technologies. The integration of organic, 2D, and 3D materials into photovoltaic and computing systems represents a significant step toward achieving global sustainability goals, particularly in reducing the environmental impact of electronic devices and supporting clean energy initiatives.

LIMITATIONS

While this study provides valuable insights into the potential of organic semiconductors, 2D materials like MoS2, and 3D materials such as perovskites, several limitations must be acknowledged to contextualize the findings and guide further investigation.

One key limitation lies in the trade-offs observed across the studied materials. For instance, perovskites demonstrated high power conversion efficiencies ($\eta \approx 21.6\%$) but exhibited relatively higher degradation rates under continuous illumination. Although recent advancements in encapsulation techniques have mitigated some stability concerns, the long-term durability of perovskite-based devices remains a challenge for practical deployment [6]. Similarly, MoS₂ showed exceptional charge-carrier mobility ($\mu \approx 200 \text{cm}^2/\text{V·s}$), but its integration into large-scale manufacturing processes is hindered by challenges related to defect density and contact resistance [11].

Organic semiconductors, while cost-effective and flexible, face limitations in terms of efficiency ($\eta \approx 11.3\%$) and operational stability. Their rapid degradation under ambient conditions (8.5% efficiency loss per 1000 hours) restricts their applicability to short-term or specialized use cases, such as disposable electronics [9]. Furthermore, the scalability of solution-based fabrication methods for organic semiconductors requires careful optimization to ensure consistent performance across large-area devices.

Another limitation pertains to the environmental impact assessment. While lifecycle assessment (LCA) metrics such as global warming potential (GWP) were used to evaluate the ecological footprint of the materials, these analyses often rely on assumptions about production processes and end-of-life scenarios. Variability in synthesis methods and regional energy mixes can introduce uncertainties in GWP estimates, necessitating more comprehensive studies to validate these results [2].

Finally, the experimental validation in this study was conducted under controlled laboratory conditions, which may not fully replicate real-world operating environments. Factors such as temperature fluctuations, humidity, and mechanical stress could influence device performance and stability, potentially altering the outcomes observed in this work.

Although the studied materials show promise as sustainable alternatives to traditional semiconductors, addressing these limitations will be critical to ensuring their practical implementation in photovoltaic and computing systems.

FUTURE DIRECTIONS

The findings of this study provide a foundation for advancing sustainable semiconductor technologies, but several opportunities remain for future research to address existing challenges and unlock the full potential of organic semiconductors, 2D materials like MoS₂, and 3D materials such as perovskites.

One promising avenue is the development of advanced encapsulation techniques to enhance the stability of perovskite-based devices. While recent progress has improved their resistance to environmental degradation, further exploration of novel barrier materials and hybrid encapsulation strategies could extend device lifetimes

under real-world conditions [6]. Additionally, investigating lead-free perovskite compositions, such as tin-based or double-perovskite structures, could mitigate toxicity concerns and broaden their applicability in eco-friendly applications.

For MoS2 and other 2D materials, future research should focus on scalable synthesis methods and defect engineering to improve material quality and device performance. Techniques such as chemical vapor deposition (CVD) have shown promise, but optimizing process parameters to reduce defect density and contact resistance remains a critical challenge [11]. Exploring heterostructures formed by stacking different 2D materials could also enable new functionalities, such as enhanced light absorption or tunable electronic properties, for photovoltaic and computing applications.

Organic semiconductors present opportunities for innovation in molecular design and processing techniques. The development of novel donor-acceptor systems with tailored energy levels could improve power conversion efficiencies beyond current benchmarks. Similarly, advancements in solution-based fabrication methods, such as inkjet printing or roll-to-roll processing, could enable cost-effective production of large-area flexible devices [3]. Efforts to enhance stability through molecular doping or cross-linking strategies may also expand their suitability for long-term applications.

Another critical direction is the integration of these materials into hybrid systems that leverage their complementary strengths. For example, combining perovskites with silicon in tandem solar cells could achieve higher efficiencies than either material alone. Similarly, incorporating MoS2 into organic semiconductor devices could enhance charge transport and overall performance. Systematic studies of hybrid architectures will be essential to identify optimal configurations and maximize synergistic effects.

Finally, expanding lifecycle assessment (LCA) frameworks to account for regional variations in energy mixes and end-of-life recycling processes could provide more accurate evaluations of environmental impact. Collaborative efforts between material scientists, engineers, and policymakers will be necessary to develop standardized metrics and guidelines for sustainable semiconductor technologies [2].

In summary, future research should prioritize addressing the limitations identified in this study while exploring innovative approaches to enhance material properties, device performance, and environmental sustainability. By pursuing these directions, the field can make significant strides toward realizing the transformative potential of green semiconductor technologies.

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