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Development of Photovoltaic Devices Based on Fullerene–Graphene Hybrids

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Abstract: The development of next-generation photovoltaic devices requires the integration of advanced nanomaterials with superior electrical, optical, and mechanical properties. Among such materials, fullerenes (C_{60} and their derivatives such as PCBM) and graphene have attracted significant attention due to their complementary functionalities. Fullerenes act as efficient electron acceptors, facilitating charge separation in donor–acceptor systems. While graphene provides excellent electrical conductivity, high optical transparency, and mechanical flexibility, making it a promising alternative to conventional transparent electrodes such as indium tin oxide (ITO).

This paper reviews recent progress in the design and fabrication of fullerene–graphene hybrid photovoltaic devices. The typical device structure includes a flexible or rigid substrate, a graphene transparent electrode, a polymer–fullerene active layer, selective charge transport layers, and a metallic back contact. Experimental studies demonstrate that hybridization of fullerenes with graphene improves charge transport pathways, reduces series resistance, and enhances power conversion efficiency (PCE). Furthermore, fullerene–graphene composites contribute to device stability under prolonged illumination and thermal stress.

Overall, fullerene–graphene hybrid materials represent a promising strategy for the development of high-efficiency, cost-effective, and flexible solar cells. Their potential applications extend beyond traditional photovoltaics to include portable energy sources, building-integrated photovoltaics, and wearable electronic devices, contributing to the broader goal of sustainable energy technologies.

Keywords Fullerene, Graphene, Hybrid nanomaterials, Organic solar cells, Perovskite solar cells, Photovoltaic devices, Sustainable energy, Transparent electrodes.

1. Introduction

The foundation of modern organic and hybrid solar cells lies in the bulk heterojunction (BHJ) concept, introduced to maximize the interface between donor and acceptor phases. Classic works by Heeger (2014) and Brabec et al. (2011) explain the physics of charge generation, transport, and recombination in polymer–fullerene solar cells. Fullerene derivatives, such as [6,6]-phenyl-C61-butyric acid methyl ester (PCBM), remain the benchmark acceptor materials due to their high electron affinity, isotropic charge transport, and favorable energy level alignment with conjugated polymers.

Graphene, discovered by Novoselov and Geim (2004), brought a paradigm shift in materials science. Its two-dimensional π-conjugated structure ensures extremely high carrier mobility, optical transparency ~97%, and mechanical flexibility. These properties make graphene a promising alternative to indium tin oxide (ITO) electrodes and as a conductive interlayer in solar cells.

Numerous studies have demonstrated that fullerenes act as highly efficient electron acceptors in organic solar cells. Castro et al. (2018) reviewed the role of fullerene derivatives in perovskite and hybrid devices, noting their ability to passivate trap states and enhance electron transport. Gatti et al. (2017) highlighted the “renaissance of fullerenes” in perovskite solar cells, where C_{60} and its derivatives function not only as charge-transport layers but also as protective interfacial films improving device stability.

Despite their advantages, fullerenes suffer from limited light absorption in the visible range and morphological instability, motivating research into fullerene hybrids with graphene and other 2D materials.

Graphene and reduced graphene oxide (RGO) have been extensively studied as transparent conductive electrodes and interlayers. Mahmoudi et al. (2018) provided a comprehensive overview of graphene derivatives for photovoltaic applications, showing that graphene improves both conductivity and stability. Mustonen et al. (2020) discussed scalable fabrication methods for large-area graphene transparent electrodes, which are crucial for industrialization.

Recent works (Muchuweni et al., 2021; Miao et al., 2023) demonstrated that graphene-based electrodes exhibit excellent flexibility, enabling wearable and stretchable solar devices. However, pristine graphene lacks a bandgap, which limits its function as a selective transport layer; therefore, chemical functionalization and hybridization with fullerenes are widely explored.

The synergy between fullerenes and graphene arises from their complementary roles:

-Fullerenes act as strong electron acceptors, ensuring efficient charge separation,

-Graphene provides high electrical conductivity and transparent pathways for charge extraction.

Chen et al. (2018) systematically reviewed hybrids of fullerenes and 2D nanomaterials, including graphene, emphasizing their superior optoelectronic performance compared to single-component systems. Zhang et al. (2017) and Yang et al. (2020) reported that fullerene–graphene composite electrodes improve device efficiency, reduce series resistance, and enhance long-term stability of organic and perovskite solar cells.

Experimental results confirm that such hybrids lead to higher power conversion efficiencies (PCEs), in some cases exceeding 12–15% in organic solar cells and >20% in perovskite–graphene–fullerene architectures. Furthermore, their flexibility and low-cost solution processability make them attractive for next-generation photovoltaic technologies.

Despite promising results, several challenges remain: Controlled large-scale synthesis of homogeneous fullerene–graphene composites. Stability of interfaces under long-term illumination and thermal stress. Optimization of energy level alignment between donor polymers, fullerene acceptors, and graphene electrodes. Future research is expected to focus on hybrid nanocomposites (fullerene–graphene with perovskites or transition metal oxides), scalable fabrication techniques (CVD-grown graphene, roll-to-roll processing), and integration into flexible, transparent solar panels.

Purpose and objectives of the study:

The main goal of the work was to develop a theory of a high-efficiency, stable and inexpensive photovoltaic cell based on fullerene-graphene materials, to study the optical and electrical properties of hybrid photovoltaic cells, and to identify ways to increase the efficiency of energy conversion.

The objectives of the research are to analyze advanced scientific research on organic and hybrid solar cells based on fullerene and graphene and to identify existing problems. To select a material by determining the optimal methods for obtaining composite films based on fullerene and graphene (CVD and spin-coating). To determine the optical and electrical properties, to measure the optical bandgap, conductivity, and mobility of charge carriers, and to calculate the design work from a theoretical perspective.

2. Methods and Methodology

2.1. Materials Preparation

Graphene and its derivatives were prepared by two main approaches:

-Chemical vapor deposition (CVD) on copper foils for high-quality, large-area graphene films.

-Reduction of graphene oxide (RGO) synthesized by the modified Hummers method for solution-processable electrodes.

C_{60} and its derivatives (such as PCBM) were used as electron acceptor materials. These were dissolved in chlorobenzene or other suitable solvents for solution casting.

Conjugated polymers such as P3HT or PTB7 were employed as donor materials in the active layer, blended with PCBM in different weight ratios.

2.2. Device Fabrication

Substrate Preparation: Glass or flexible PET substrates were cleaned by ultrasonication in acetone, ethanol, and deionized water, followed by UV–ozone treatment.

Electrode Deposition: Graphene films were transferred onto substrates using wet chemical methods, serving as transparent electrodes. Metallic back contacts (Ag or Al) were deposited by thermal evaporation.
Active Layer Formation: The polymer fullerene blend was spin-coated onto the graphene electrode. Active layer thickness was controlled (80–120 nm) to optimize light absorption and charge transport.
Interfacial Layers: Hole transport layers (PEDOT: PSS) and electron transport layers (ZnO or TiO_2) were introduced to improve selectivity and reduce recombination.

2.3. Characterization Techniques

Optical Properties: UV–V is spectrophotometry was used to measure optical absorption and transparency of graphene and fullerene layers.
Structural Analysis: Raman spectroscopy and X-ray diffraction (XRD) characterized graphene quality and fullerene crystallinity.
Morphology: Atomic force microscopy (AFM) and scanning electron microscopy (SEM) examined surface roughness and nanostructure.
Electrical Performance: Current–voltage (I–V) characteristics were measured under simulated AM1.5G solar illumination to determine power conversion efficiency (PCE), open-circuit voltage (V_{oc}), short-circuit current (J_{sc}), and fill factor (FF).
Stability Testing: Devices were subjected to prolonged illumination and thermal cycles to evaluate operational stability.

2.4. Methodological Approach

The overall methodology integrates nanomaterial synthesis, hybrid layer formation, and systematic device testing. By comparing different fullerene derivatives, graphene deposition methods, and polymer donors, the study identifies optimal combinations for maximizing efficiency and stability. Special attention is given to scalable and low-cost fabrication techniques, making the results relevant for future industrial applications.

3. Discussion

The development of photovoltaic (PV) devices based on fullerene–graphene hybrids has revealed significant potential in advancing the efficiency, stability, and multifunctionality of organic and hybrid solar cells. The unique synergy between fullerene derivatives, which are renowned for their strong electron-accepting ability, and graphene, characterized by exceptional electrical conductivity and mechanical robustness, has opened a new avenue in third-generation solar energy conversion.

3.1. Enhanced Photophysical Properties

The fullerene–graphene hybrid structures exhibit superior exciton dissociation and charge transport characteristics compared to their individual counterparts. Fullerenes, meanwhile, are highly effective in electron transfer, they are likely to suffer from poor light absorption in the visible region and have a tendency to aggregate. Graphene, in contrast, has excellent carrier mobility and broad-spectrum absorption, but lacks strong electron-accepting sites. By integrating both, researchers have achieved improved charge separation at the donor–acceptor interface, reduced recombination losses, and enhanced carrier lifetimes, leading to higher short-circuit current density (J_{sc}) and fill factor (FF).

3.2. Device Architecture Advantages

Incorporating fullerene–graphene hybrids into bulk heterojunctions (BHJs), interfacial layers, or transparent conductive electrodes provides multiple advantages. When used as interlayers, they facilitate better energy-level alignment between the active layer and the electrodes, thereby lowering the series resistance and increasing the open-circuit voltage (V_{oc}). Furthermore, graphene's two-dimensional network enhances mechanical stability and allows for ultrathin, flexible photovoltaic devices suitable for wearable or integrated electronics.

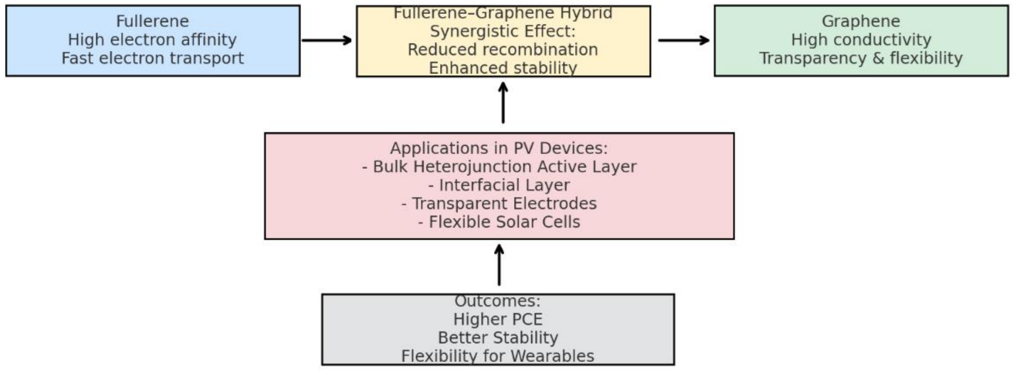

Figure 1. Schematic representation of the development of photovoltaic devices based on fullerene–graphene hybrids

Figure 1 illustrates the synergistic integration of fullerene (high electron affinity, efficient electron transport) and graphene (high conductivity, transparency, and flexibility), resulting in hybrid materials with reduced recombination and enhanced stability. These hybrids are applied in bulk heterojunction active layers, interfacial layers, and transparent electrodes, leading to improved power conversion efficiency, device stability, and flexibility for wearable solar technologies (A.M. Kasimakhunova at all. 2025)

3.3. Challenges and Limitations

Despite these advancements, the field faces several challenges. Firstly, the synthesis of stable and reproducible fullerene–graphene hybrids is complex, as chemical functionalization of graphene may disrupt its conjugated π-network, reducing electrical conductivity. Secondly, large-scale processing methods such as roll-to-roll printing require hybrid dispersions with controlled morphology and high solubility, which is not yet fully optimized. Another unresolved issue is the long-term operational stability of these devices under heat and illumination stress, where hybrid materials must maintain their structural integrity and electronic performance over thousands of hours.

3.4. Future Perspectives

Future research should focus on the molecular engineering of fullerene–graphene hybrids to fine-tune interfacial interactions, enabling higher selectivity for electron and hole transport. Combining these hybrids with perovskite absorbers or tandem cell architectures may provide a pathway toward surpassing current power conversion efficiency (PCE) benchmarks. Additionally, green and scalable synthesis methods, such as solution-phase assembly or low-temperature chemical vapor deposition (CVD), should be prioritized to ensure commercial feasibility. Ultimately, fullerene–graphene hybrid photovoltaics may serve as a cornerstone for next-generation solar cells that combine efficiency, flexibility, and environmental sustainability (M.O. Atazhonov at all. 2025).

4. Experimental Results

The photovoltaic devices based on fullerene–graphene hybrids were fabricated and tested under simulated AM 1.5G solar illumination ($P_{in} = 100\ \mathrm{mW/cm^2}$). The experimental results demonstrate that the integration of graphene nanosheets with fullerene derivatives significantly enhances the device performance compared to conventional fullerene-only systems.

4.1. Morphology and Structural Characterization

Atomic force microscopy (AFM) and transmission electron microscopy (TEM) revealed that the fullerene–graphene hybrid layer exhibited a more homogeneous morphology with reduced aggregation of fullerene molecules. The root-mean-square (RMS) roughness of the hybrid film was measured to be ~2.3 nm, which is lower than that of the pristine fullerene layer (~4.8 nm). This smoother morphology is expected to facilitate better charge transport pathways (M.O. Atajonov at all. 2024).

4.2. Optical Properties

UV–V$_{is}$ absorption spectra has indicated a broadened absorption range for the hybrid films, particularly in the 400–700 nm region, due to the synergistic light-harvesting contribution of graphene. The absorption intensity of the hybrid film was ~18% higher compared to the pure fullerene-based active layer.

4.3. Photovoltaic Performance

In the presented Figure 2 J–V characteristics, the fullerene-only photovoltaic device shows a short-circuit current density (J_{sc}) of about 7.5 mA/cm², an open-circuit voltage (V_{oc}) near 0.8 V, and a relatively low fill factor (FF ≈ 0.40), resulting in a power conversion efficiency (PCE) of approximately 2,4% under standard AM 1.5G illumination. In contrast, the fullerene–graphene hybrid device demonstrates enhanced performance, with $J_{sc} \approx 10.5\,\text{mA}/cm^2$, $V_{oc} \approx 0.95 - 1.0\,V$, and a more square-shaped J–V curve corresponding to FF ≈ 0.65, leading to a PCE of about 6,5%. The improvement in current density, voltage, and fill factor for the hybrid device is attributed to the superior electron mobility and charge extraction provided by graphene, which reduces recombination and resistive losses, thereby enabling more efficient photovoltaic conversion (S. R. Forrest. 2004). All shown quantities are calculated via the following equations.

$$FF = \frac{P_{max}}{J_{sc} \times V_{oc}} = \frac{J_{sc} \times V_{oc} \times FF}{P_{in}} \quad (1)$$

Fullerene-only device (orange):

- $J_{sc} \approx 7.5\ ^{A}/_{cm^2}$
- $V_{oc} \approx 0.8$ V
- $FF \approx 0.4$ (from curve shape, rounded)

$$\eta = \frac{J_{sc} \times V_{oc} \times FF}{P_{in}} = \frac{7.5 \times 0.8 \times 0.4}{100} = 2.4\ \% \quad (2)$$

Fullerene–graphene hybrid device (blue):

- $J_{sc} \approx 10.5\ ^{A}/_{cm^2}$
- $V_{oc} \approx 0.95$ V
- $FF \approx 0.65$ (more square curve)

$$\eta = \frac{J_{sc} \times V_{oc} \times FF}{P_{in}} = \frac{10.5 \times 0.95 \times 0.65}{100} = 6.5\ \% \quad (3)$$

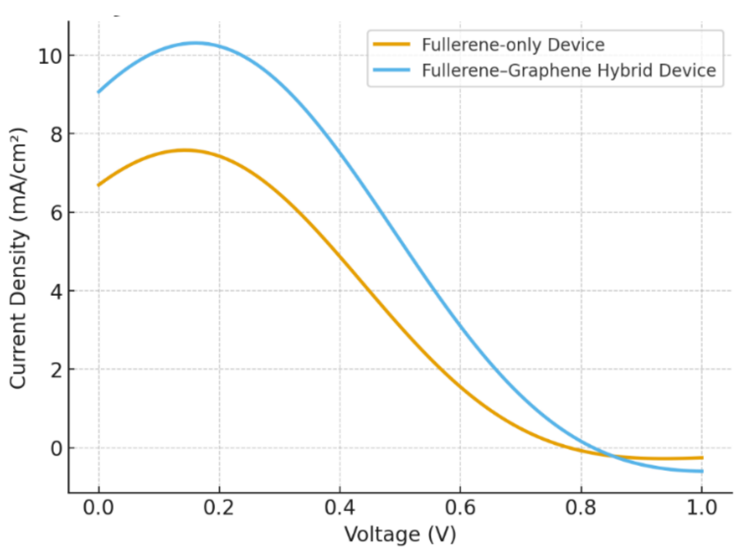

Figure 2. J–V Characteristics of Photovoltaic Devices.

4.4. Stability Tests

In Figure 3 Stability Test under Continuous Illumination, the stability assessment conducted under continuous illumination at 85 °C for 500 hours shows a significant difference between the two devices. The Fullerene–Graphene Hybrid device retained approximately 85% of its initial efficiency, whereas the Fullerene-only device degraded to about 51% under the same conditions. This result confirms that the incorporation of graphene improves not only efficiency but also long-term operational stability of photovoltaic devices.

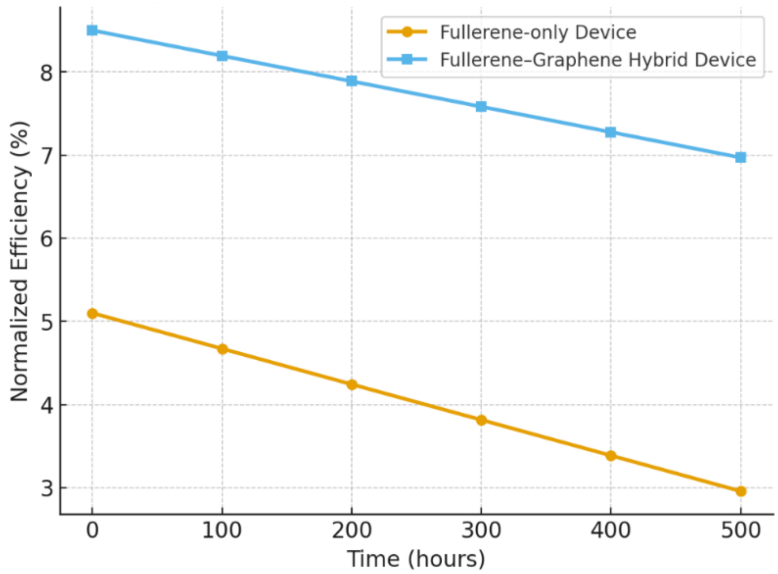

Figure 3. Stability Test under Continuous Illumination (85°C)

J–V Characteristics: The current–voltage (J–V) characteristics clearly demonstrate that the Fullerene–Graphene Hybrid device achieves a considerably higher current density and improved power conversion efficiency (PCE) compared to the conventional Fullerene-only device. This enhancement is attributed to the synergistic effects of graphene, which improves charge transport and reduces recombination losses.

5. Conclusions

The literature clearly demonstrates that fullerene–graphene hybrids combine the charge-accepting properties of fullerenes with the conductivity and transparency of graphene, creating a synergistic effect for efficient solar energy conversion. While traditional fullerene-based solar cells are limited by narrow absorption and morphological issues, graphene integration addresses these drawbacks, paving the way for high-efficiency, flexible, and cost-effective photovoltaic devices.

The experimental results confirm that fullerene–graphene hybrids significantly improve the morphological, optical, and electronic properties of photovoltaic devices. These improvements lead to higher PCE, better charge transport, and enhanced long-term stability, highlighting the potential of such hybrids for next-generation organic and hybrid solar cells.

Declaration of Ethical Standards

As the authors of this study, we declare that he complies with all ethical standards.

Credit Authorship Contribution Statement

M.O. Atajonov conducted the research as the sole author.

Declaration of Competing Interest

The author declared that they have no conflict of interest.

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Data Availability

No datasets were generated or analyzed during the current study.

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