Materials Science

Query paper:
Title: Organic solar cells based on non-fullerene acceptors
Abstract: Organic solar cells (OSCs) have been dominated by donor:acceptor blends based on fullerene acceptors for over two decades. This situation has changed recently, with non-fullerene (NF) OSCs developing very quickly. The power conversion efficiencies of NF OSCs have now reached a value of over 13%, which is higher than the best fullerene-based OSCs. NF acceptors show great tunability in absorption spectra and electron energy levels, providing a wide range of new opportunities. The coexistence of low voltage losses and high current generation indicates that new regimes of device physics and photophysics are reached in these systems. This Review highlights these opportunities made possible by NF acceptors, and also discuss the challenges facing the development of NF OSCs for practical applications.

Candidate papers:

1. **Title:** Fullerene-Free Polymer Solar Cells with over 11% Efficiency and Excellent Thermal Stability.
   Abstract: A nonfullerene-based polymer solar cell (PSC) that significantly outperforms fullerene-based PSCs with respect to the power-conversion efficiency is demonstrated for the first time. An efficiency of> 11%, which is among the top values in the PSC field, and excellent thermal stability is obtained using PBDB-T and ITIC as donor and acceptor, respectively.
2. **Title:** Fast charge separation in a non-fullerene organic solar cell with a small driving force
   Abstract: Fast and efficient charge separation is essential to achieve high power conversion efficiency in organic solar cells (OSCs). In state-of-the-art OSCs, this is usually achieved by a significant driving force, defined as the offset between the bandgap (E gap) of the donor/acceptor materials and the energy of the charge transfer (CT) state (E CT), which is typically greater than 0.3 eV. The large driving force causes a relatively large voltage loss that hinders performance. Here, we report non-fullerene OSCs that exhibit ultrafast and efficient charge separation despite a negligible driving force, as E CT is nearly identical to E gap. Moreover, the small driving force is found to have minimal detrimental effects on charge transfer dynamics of the OSCs. We demonstrate a non-fullerene OSC with 9.5% efficiency and nearly 90% internal quantum efficiency despite a low voltage loss of 0.61 V. This creates a path towards highly efficient OSCs with a low voltage loss.
3. **Title:** Breaking the 10% efficiency barrier in organic photovoltaics: Morphology and device optimization of well-known PBDTTT polymers
   Abstract: With the advances in organic photovoltaics (OPVs), the invention of model polymers with superior properties and wide applicability is of vital importance to both the academic and industrial communities. The recent inspiring advances in OPV research have included the emergence of poly(benzodithiophene-co-thieno[3,4-b]thiophene) (PBDTTT)-based materials. Through the combined efforts on PBDTTT polymers, over 10% efficiencies have been realized recently in various types of OPV devices. This review attempts to critically summarize the recent advances with respect to five well-known PBDTTT polymers and their design considerations, basic properties, photovoltaic performance, as well as device application in conventional,

inverted, tandem solar cells. These PBDTTT polymers also make great contributions to the rapid advances in the field of emerging ternary blends and fullerene-free OPVs with top performances.

4. **Title:** Vibrational coherence probes the mechanism of ultrafast electron transfer in polymer–fullerene blends
   Abstract: The conversion of photoexcitations into charge carriers in organic solar cells is facilitated by the dissociation of excitons at the donor/acceptor interface. The ultrafast timescale of charge separation demands sophisticated theoretical models and raises questions about the role of coherence in the charge-transfer mechanism. Here, we apply two-dimensional electronic spectroscopy to study the electron transfer process in poly(3-hexylthiophene)/PCBM (P3HT/PCBM) blends. We report dynamics maps showing the pathways of charge transfer that clearly expose the significance of hot electron transfer. During this ultrafast electron transfer, vibrational coherence is directly transferred from the P3HT exciton to the P3HT hole polaron in the crystalline domain. This result reveals that the exciton converts to a hole with a similar spatial extent on a timescale far exceeding other photophysical dynamics including vibrational relaxation.
5. **Title:** Ultrafast Long-Range Charge Separation in Organic Semiconductor Photovoltaic Diodes
   Abstract: In photovoltaic devices, electrons excited by the absorption of light must travel across a junction, while the positively charged “holes” they leave behind effectively migrate in the opposite direction. If the electrons and holes do not separate efficiently, they can recombine and fail to produce any appreciable current. Gélinas studied this separation process by ultrafast optical absorption spectroscopy in thiophene-derived donor-fullerene acceptor systems common in organic photovoltaics and report a rate significantly faster than simple charge diffusion would suggest. The results implicate a coherent charge delocalization process, likely to involve fullerene π-electron states.
6. **Title:** Conjugated-polymer blends for optoelectronics
   Abstract: Solution-processed polymer optoelectronic devices such as light-emitting diodes and solar cells have many advantages for large-area manufacture, and show increasing levels of performance. Here, we review recent progress in using blends of two conjugated polymers for optoelectronic devices. The blending of two or more polymers allows tuning of device performance, and for photovoltaics presents an attractive way to combine donor and acceptor materials with a morphology controlled by polymer phase separation. We discuss recent advances in imaging the microstructure of conjugated polymer blends, and we demonstrate how the blend structure leads to performance advantages in both LEDs and photovoltaic devices.

Exemplary analysis:

1. **Relevance:** It supports the query paper's claim about the advancements in non-fullerene OSCs, showcasing their potential over traditional fullerene-based OSCs.
   Reason for Citation: This paper is likely cited as an example of the significant progress in the field of non-fullerene OSCs, demonstrating high power conversion efficiency and excellent thermal stability.
2. **Relevance:** It highlights the achievement of high efficiency and low voltage loss in non-fullerene OSCs, which is a critical aspect of the new opportunities mentioned in the query paper.

Reason for Citation: The query paper might reference this study to discuss the advancements in charge separation mechanisms in non-fullerene OSCs.

3. **Relevance:** It might be used to contextualize the progress in non-fullerene OSCs within the broader advancements in organic photovoltaic materials and device optimization.
   Reason for Citation: This review could be cited to provide a background on the significant milestones in the field of organic photovoltaics, particularly the breaking of the 10% efficiency barrier.
4. **Relevance:** This could serve as a contrast to the mechanisms at play in non-fullerene OSCs or to highlight areas where further understanding is needed in the context of NF acceptors.
   Reason for Citation: Although this paper focuses on fullerene blends, it might be cited in the query paper to discuss the fundamental mechanisms of electron transfer and the role of vibrational coherence.
5. **Relevance:** It may be used to underline the importance of efficient charge separation in achieving high performance in OSCs, including those based on non-fullerene acceptors.
   Reason for Citation: This study is likely referenced to discuss the principles of charge separation in organic semiconductor devices.
6. **Relevance:** It might be used to discuss the potential of blending techniques in optimizing the morphology and performance of non-fullerene OSCs, aligning with the opportunities for device physics and photophysics advancements mentioned in the query paper.
   Reason for Citation: This review could be cited to provide an overview of the use of conjugated-polymer blends in optoelectronics, including solar cells.

Exemplary ranking: Ranked order: paper 1, paper 2, paper 3, paper 6, paper 5, paper 4

1. **Explanation:** This paper directly addresses the core advancements in non-fullerene OSCs, which is the primary focus of the query paper. Its emphasis on efficiency and thermal stability is crucial for practical applications, making it highly relevant for further research in improving non-fullerene OSCs.
2. **Explanation:** The mechanism of charge separation is fundamental to the efficiency of OSCs. This paper's focus on achieving fast charge separation with a small driving force in non-fullerene OSCs is directly relevant to overcoming challenges in device physics, a key theme in the query paper.
3. **Explanation:** This paper provides a broader context on the milestones in organic photovoltaics, including efficiency improvements. It is relevant for understanding the historical progress and the significance of surpassing the 10% efficiency barrier, which is a benchmark for the advancements in non-fullerene OSCs discussed in the query paper.
4. **Explanation:** Although this paper focuses on fullerene blends, its exploration of electron transfer mechanisms can provide a comparative background or foundational knowledge that might be applicable to non-fullerene systems. It is ranked last due to its indirect relevance to the specific focus on non-fullerene acceptors.
5. **Explanation:** Understanding the principles of charge separation is essential for all OSCs. This paper's relevance comes from its discussion on the efficiency of charge separation, which is a critical factor for the performance of non-fullerene OSCs.

6. **Explanation:** The review on conjugated-polymer blends for optoelectronics, including solar cells, offers insights into material science and engineering aspects that are crucial for optimizing non-fullerene OSCs. It is relevant for exploring new opportunities in device physics and photophysics advancements.