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## Supporting information

# Challenges and Limitations of ChatGPT and Artificial Intelligence for Scientific Research: A Perspective from Organic Materials

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**Supporting Information S1.** The response from ChatGPT when asking “List the most popular research directions for organic solar cells”

Organic solar cells are an active area of research with many potential applications in renewable energy, electronic devices, and other fields. Here are some of the most popular research directions for organic solar cells:

**Material Development:** The development of new materials is a key area of research in organic solar cells. Researchers are working to identify and synthesize new organic compounds, such as polymers and small molecules, that can efficiently absorb sunlight and transport charge carriers. This includes exploring new conjugated polymers, non-fullerene acceptors, and perovskite materials.

**Device Optimization:** Another important area of research is the optimization of the device architecture and processing conditions to improve the performance and stability of organic solar cells. This includes developing new device structures and interface engineering techniques, as well as optimizing the device geometry, electrode materials, and other parameters to improve the power conversion efficiency, stability, and scalability of organic solar cells.

**Tandem and Hybrid Devices:** Tandem and hybrid devices combine multiple absorbers and charge transport layers to achieve higher efficiencies and stability. Research in this area is focused on developing new materials and device architectures for tandem and hybrid organic solar cells, as well as exploring the potential of using organic and inorganic materials in combination.

**Large Area and Flexible Devices:** Organic solar cells can be fabricated on flexible and lightweight substrates, making them ideal for large area applications, such as building-integrated photovoltaics and wearable electronics. Research in this area is focused on developing new materials and device architectures that can be fabricated on flexible substrates, as well as exploring the potential of using solution-based and roll-to-roll processing techniques for scalable production.

**Stability and Durability:** The stability and durability of organic solar cells are important factors for their commercial viability. Research in this area is focused on understanding the degradation mechanisms of organic solar cells and developing new materials and device architectures that can improve the stability and lifetime of organic solar cells. This includes exploring the use of encapsulation techniques, new electrode materials, and other strategies to protect organic solar cells from environmental factors, such as moisture, oxygen, and UV radiation.

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**Supporting Information S2.** The response from ChatGPT when asking “Give me more details on the materials aspect”.

The development of new materials is a crucial area of research in organic solar cells, as the performance and efficiency of the cells are directly influenced by the properties of the materials used. The most commonly used materials in organic solar cells are conjugated polymers and fullerene derivatives, but researchers are also exploring other materials, such as non-fullerene acceptors, perovskites, and other inorganic/organic hybrid materials.

**Conjugated Polymers:** Conjugated polymers are a class of materials that exhibit high optical absorption and charge mobility, making them ideal for use as the active layer in organic solar cells. Researchers are working to develop new conjugated polymers with improved properties, such as broader absorption spectra, higher charge mobility, and better stability. This includes exploring new chemical structures, functional groups, and processing techniques to optimize the properties of the polymers.

**Non-Fullerene Acceptors:** Fullerene derivatives have traditionally been used as electron acceptors in organic solar cells, but their limited absorption spectra and high cost have led researchers to explore alternative materials. Non-fullerene acceptors (NFAs) are a new class of organic materials that exhibit high absorption coefficients and electron mobility, making them ideal for use as electron acceptors in organic solar cells. Researchers are working to develop new NFAs with improved properties, such as broader absorption spectra, higher electron mobility, and better stability.

**Perovskites:** Perovskites are a class of inorganic materials that exhibit excellent optical and electronic properties, including high absorption coefficients and long carrier lifetimes. Perovskite solar cells have shown high power conversion efficiencies and are emerging as a promising alternative to traditional organic solar cells. Researchers are working to develop new perovskite materials with improved stability and scalability, as well as exploring the potential of using perovskite materials in tandem and hybrid solar cells.

**Other Materials:** Researchers are also exploring other organic and inorganic materials for use in organic solar cells, such as small molecule acceptors, graphene, carbon nanotubes, and metal oxide nanoparticles. These materials offer unique properties and have the potential to improve the efficiency, stability, and scalability of organic solar cells.

**Supporting Information S3.** The response from ChatGPT when asking “Why polymers mobility is higher than small molecules mobility”

The mobility of a material is related to its ability to transport charge carriers (electrons or holes) under an applied electric field. In the case of organic semiconductors, the mobility is determined by the ability of the material to form a continuous pathway of overlapping molecular orbitals, which allows charge carriers to move through the material.

Polymers are typically more disordered and have a lower degree of crystallinity compared to small molecules, which can lead to a higher degree of disorder in the molecular packing. However, this disorder can also result in more amorphous regions that facilitate the mobility of charge carriers through the material. Additionally, polymers can form more extensive and interconnected networks, which can provide more pathways for charge carrier transport.

In contrast, small molecules tend to have a more ordered and crystalline structure, which can lead to more efficient exciton generation and transport. However, this can also lead to more defects and trap states in the material, which can hinder the mobility of charge carriers.

Overall, the higher mobility of polymers compared to small molecules can be attributed to their more disordered and amorphous nature, which allows for more efficient charge carrier transport through the material.