POLYMER SOLAR CELLS FROM DIBLOCK COPOLYMERS: A COMPUTATIONAL INVESTIGATION OF SELF-ASSEMBLED COPOLYMERS

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Abstract

Current silicon based solar cell technologies have proven to be inordinately expensive to manufacture relative to the power that they are capable of generating, however the power for clean energy production remains high. In contrast, polymer solar cells may be produced cheaply, albeit at a significantly reduced photovoltaic efficiency. Comparatively modest gains in efficiency may push polymer solar cells into the realm of economic feasibility and potentially even superease silicon based solutions.

This research details a novel algorithm to model the principle charge transport mechanisms and photovoltaic properties of polymer solar cells. The algorithm is utilized to measure the quantum efficiency of common and complex diblock copolymer morphologies via the Monte Carlo method is easily extensible to further morphological analyses. This research serves as the foundation for future investigations that will seek to optimize photovoltaic generation with the aid of terminal predictions that guide solar cell architectures which may significantly improve photovoltaic production in polymer based solar cells.

Principles and Components of Polymer Solar Cells

Solar cells convert usable energy from sunlight by utilizing the energy carried by that light to drive current (Fig.1). Photovoltaic efficiency is a fundamental metric to the field which essentially compares the amount of light electrons to the amount of electrons extracted, and thereby provides a general indication of the efficiency of a solar cell.

The cell itself is composed of two main components, a donor polymer, and an acceptor polymer. The donor polymer absorbs the light and creates an electron-hole pair, while the acceptor polymer assists in the separation of the charges. The separation of the charges ultimately results in a voltage difference, which can be converted into electricity.

The pathways followed by excitons and the resultant electron-hole pairs, as well as the factors affecting their movement, are the key components to optimizing photovoltaic production. The efficiency of the cell is dependent on the probability of exciton dissociation and its ability to reach proper locations for extraction before recombination occurs.

The probability of exciton dissociation and the efficiency of the cell itself are a result of the morphology of the cell. The morphology refers to the arrangement of the polymer chains within the cell, and it significantly affects the efficiency of the cell.

Efficiency is determined by both the probability of exciton dissociation and the mobility of the charge carriers. The charge carriers are subjected to various forces, including thermal fluctuations and electric fields, which can affect their movement and the efficiency of the cell.

The efficiency of polymer solar cells can be optimized by improving the morphology of the cell, which can be achieved through various techniques such as blending, doping, and thermal treatment. These techniques can alter the arrangement of the polymer chains, thereby improving the efficiency of the cell.

Results and Discussions

In considering two significant test cases—a classical homogeneous bilayer geometry and a more realistic interfaceless diblock diblock polymer (Fig. 2 A and B respectively)—many of the critical factors affecting photovoltaic cell efficiency are elucidated.

For this reason it is evident that the photovoltaic efficiency of polymer solar cells can be attributed to the efficiency of the cell itself, which is strongly influenced by the morphology of the cell.

The efficiency of polymer solar cells is significantly lower than that of traditional photovoltaic technologies. This is primarily due to the relatively low efficiency of the polymer solar cells, despite their lower cost of production.

The efficiency of polymer solar cells can be improved by optimizing the morphology of the cell. This can be achieved through various techniques such as blending, doping, and thermal treatment, which can alter the arrangement of the polymer chains, thereby improving the efficiency of the cell.

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