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Novel Organic and Polymeric Materials for Solar Energy Conversions

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Abstract

Organic or ‘plastic’ solar cells are attractive for solar photoelectric energy conversion applications where low cost (such as large area), lightweight, and flexible shape are desired. The photoelectric power conversion efficiencies of currently reported organic/polymeric photovoltaic materials are still relatively low (typically less than 10% under AM 1.5 and one Sun intensity), and the three major losses are still severe, *i.e.*, the ‘photon loss’ due to mismatch of materials energy gaps versus the sunlight photon energies, the ‘exciton loss’ and the ‘carrier loss’ due to poor solid state morphologies of existing polymeric donor/acceptor binary systems. Therefore, both molecular frontier orbitals (HOMOs, LUMOs) and phase morphologies need to be engineered to further enhance the efficiency. In this paper, our recent efforts on frontier orbital and energy gap engineering and terminal functionalizations of conjugated polymer blocks, and a donor-bridge-acceptor type block copolymer approach will be reviewed. For instance, a new donor-bridge-acceptor or DBA type conjugated block copolymer system has been successfully synthesized, characterized, and solar cells based on the new materials has been preliminarily tested revealing better performance of the block copolymer system versus the donor/acceptor simple blend system. In addition, dye sensitized polymer and organic/inorganic hybrid nanostructure solar cells were also investigated as dyes absorb more sunlight photon and have more available energy levels and gaps that can better match the solar spectrum than traditional solar cells.

Keywords: Organic solar cells; polymer solar cells; block copolymers; dye solar cells; triple component system, optoelectronic devices; solar energy; frontier orbitals; HOMO, LUMO, absorption coefficients.

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1. Introduction

Widespread use of inorganic based solar cell technology as an alternative energy source are still limited due to the high cost or high energy consumption associated with the elaborate fabrication processes involving elevated temperature, high vacuum, as well as a current shortage of feedstock materials [1-3]. Organic and polymeric solar cells offer many competitive advantages, including convenient fine tuning of materials chemical structures, frontier orbitals (HOMOs and LUMOs), energy gaps (E_g), materials durability, and low cost and versatility for solution-based large-scale industrial processing and fabrications, including well-established polymer solution printing techniques or a roll-to-roll (R2R) thin film processing protocol [4-8]. In addition, organic and polymeric semiconductors exhibit much higher optical absorption coefficients compared to their inorganic counter-parts, thus opening possibilities for the production of very thin solar sheets or films that could save large amount of materials [8]. The current best reported polymer based solar cell has a power conversion efficiency of about 8-10% under one Sun at AM 1.5 [9-11], the cells typically contain a blend of donor type polymer with an acceptor (generally fullerene derivatives). However, fullerenes are not cost effective yet, and the morphology (such as donor/acceptor phase domain size and ordering) of a physical blend is not easy to control.

The critical success factors for organic and polymeric solar cells include the improvement of photon capture via energy gap engineering, particularly in the most intense sunlight radiations of 1-2 eV, and the improvement of charge generation and transport via polymer morphology engineering, as it is now clear that the photo induced charge separation is critically affected by the donor/acceptor domain size, and charge mobility is critically affected by the polymer morphology [4-11].

The overall photoelectric power conversion efficiency of an organic/polymeric solar cell is determined by at least following five critical steps [4-5]:

- 1) Photon capture or exciton generation;
- 2) Exciton diffusion to donor/acceptor interface;
- 3) Exciton dissociation or carrier generation at donor/acceptor interface;
- 4) Carrier diffusion to respective electrodes;
- 5) Carrier collection by the respected electrodes.

So far none of the five steps have been optimized, which accounts for the relatively low power conversion efficiencies of organic photovoltaics (the best reported/announced efficiency is about 10% [11]). However, all these five steps can be and should be improved via systematic improvements on materials design, synthesis, processing, and fabrications.

In the first step of photon capture (also occurring in the photo synthesis of natural plants), a basic requirement is that the materials optical excitation energy gap (E_g) must match the incident photon energy. In most organic materials, the energy gap defaults to the difference between the HOMO (highest occupied molecular orbital) and the LUMO (lowest unoccupied molecular orbital) frontier orbital levels.

For terrestrial solar cell applications, it is desirable that the energy gaps of the materials span a broad range of 1.0-2.0 eV. Many widely used conjugated semiconducting polymers used in organic solar cell have energy gaps bigger than 2.0 eV. This is why the photon capture for organic PV cells still needs to be optimized at AM 1.5. This 'photon loss' problem is in fact very common in most of the currently reported

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