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REGULAR ARTICLE

Electron Transfer Pathways in the Z-schematic Donor-donor-acceptor Organic Solar Cells

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Abstract: In the tandem organic solar cell, two or more subcells are generally connected in series to generate a high open circuit voltage by using an interlayer for charge carrier recombination. In this communication, a donor-donor-acceptor organic solar cell model without the interlayer is suggested for generation of high open circuit voltage. The mechanism of this model, similar to the Z-scheme, requires that both of two donors absorb sunlight step-by-step to perform a high energy charge transfer state. Although there are many competitive electron transfer (ET) processes taking place between two donors after photo excitations, the possibility of this mechanism is theoretically demonstrated by using electronic structure calculations and Marcus ET theory from a model solar cell where the substituent of DFHCO4TCO and P3DOT are taken as donors, and $PC_{61}BM$ as an acceptor. It is found that the obtained open circuit voltage is twice as large as that in the organic solar cell with single donor.

AMS subject classifications: 65D18, 68U05

Key words: donor-donor-acceptor organic solar cells, electron transfer, Z-scheme, open circuit voltage, driving force, substituent

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1 Introduction

Organic photovoltaic devices are becoming one of potential candidates in the solar cells for their low-cost, flexibility, ease of processing and low toxicity [1-3]. An organic solar cell typically consists of p-type (donor) and n-type (acceptor) semiconductors, interfaced in a bulk heterojunction (BHJ) configuration, and its open-circuit voltage (V_{oc}) is one of significant factors to determine the power conversion efficiency[4, 5]. The experiments have demonstrated that V_{oc} displays a linear relationship with the energy gap between the ionization potential of donor and electronic affinity of acceptor [6-8]. This energy gap essentially corresponds to the energy difference between the highest occupied molecular orbital (HOMO) of donor and the lowest unoccupied molecular orbital (LUMO) of acceptor [9]. Accordingly, the weak donor- strong-acceptor strategy has been proposed to design the polymer donor in the solar cell with a large V_{oc}, where the strong-acceptor part of the polymer is used to reduce the band gap and the weak-donor part keeps the HOMO energy at a low level [10, 11]. To further improve the conversion efficiency, organic tandem solar cells have been designed to achieve higher overall solar absorption [12-16]. In this kind of solar cells, two subcells are stacked via an interlayer for the charge recombination. Meanwhile, with the series connection of two subcells, the open circuit voltage of an ideal tandem solar cell should equal to the sum of those of the subcells. Based on the rule to produce the tandem solar cell with a high V_{oc}, where the electron and hole recombine at the interlayer, one may get an inspiration that when the HOMO and LUMO energy levels in two donors match well, the excited electron in the LUMO of the left donor and the hole in the HOMO of the right one may also recombine in the D-D-A solar cell. With this scheme, the V_{oc} might be doubly enlarged compared to that of the D-A solar cell. Indeed, the similar mechanism, known as Z-scheme, has been confirmed by the experiments of artificial photosynthesis, photocatalytic reactions and etc[17-21], where the systems are pumped step-by-step to the high excited states. In this paper, we theoretically illustrate the possibility of the Z-schematic D-D-A solar cell through electronic structure calculations and Marcus ET theory[22, 23].

2 Model