Commun. Comput. Chem
doi: 10.4208/cicc.2017.v5.n4.3

Vol.5, No.4, pp.121-136
Dec 2017

Regular Article

A theoretical research on the impact of pyridine based and fused cyclic based polymer on the properties of donor polymer for organic solar cells

Yalin Ran, Xian Peng, Xiaoqin Tang, Xiaorui Liu, Wei Shen, Rongxing He, Ming Li*

Key Laboratory of Luminescence and Real-Time Analytical Chemistry (Southwest University), Ministry of Education, College of Chemistry and Chemical Engineering, Southwest University, Chongqing 400715, China.

Received 15 Nov. 2017; Accepted (in revised version) 25 Dec. 2017

Abstract: The polymer with D-A structure has been certified a significant role as donor materials of organic solar cells (OSCs) for its outstanding light absorption. In this work, the properties of pyridine based and fused cyclic based D-A polymer was studied by means of DFT and TD-DFT theory under PBE0/6-31G(d) level. Based on the reported polymer D1, pyridine and fused cyclic were introduced to D2, D3 and D4. Compared with polymer lacking the pyridine and fused cyclic, the pyridine and fused cyclic based exhibits better planarity, lower HOMO energy and broader absorption properties, which are helpful to get a higher V_{oc} and J_{sc}. Moreover, fused cyclic based as well as pyridine monocycle and pyridine fused cyclic based polymer shows the ability to enhance the hole transfer rate. Hence, the approach of introducing pyridine and fused cyclics to polymer donor is a feasible way to modulate the electron-withdrawing capability in D-A polymer chain thereby promotes the performance of the OPV devices.

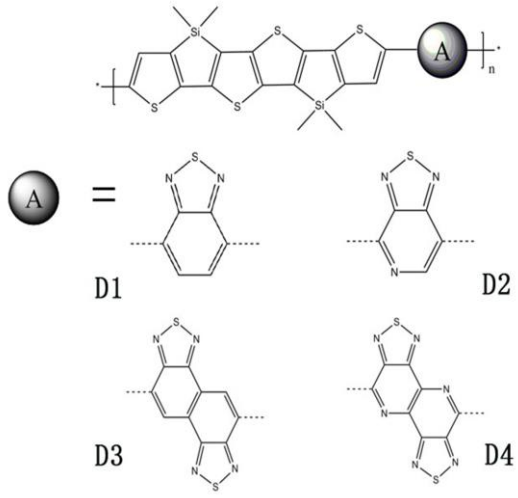
Keywords: Organic solar cells, density functional theory, D-A polymer, DFT, TD-DFT, absorption

* Corresponding author. *E-mail address*: liming@swu.edu.cn(Ming Li)

1. Introduction

Polymer solar cells (PSCs) possess desirable characteristic such as low cost, flexibility and lightweight attracting much attention from academia [1]. In bulk-heterojunction solar cells (BHJSCs), the phase-separated donor/acceptor blend layer is constituted of conjugated polymers, and fullerene derivatives like [6,6]-phenyl-C61-butyric acid methyl ester (PC61BM) or [6,6]-phenyl-C71-butyric acid methyl ester (PC71BM) traditionally [2]. The D-A conjugated copolymers donor material in typical BHJSCs always comprises of electron rich moieties (donor, D) and electron deficient moieties (acceptor, A) [3]. A remarkable amount of effort in the past decades have made to improves the power conversion efficiency of BHJSCs largely. The state-of-the-art PCE of single-junction BHJSCs has been exceeded 10% and their tandem counterparts can achieve more in many research groups report recently. Such as jing bozhao et al. achieved a PCE of 11.7% by polymer donor material PffBT4T-C9H13 successfully.

In OPV devices, the open circuit voltage (V_{oc}), short-circuit current density (J_{sc}) and the fill factor (FF) are related to the power conversion efficiency (PCE). V_{oc} is related to the difference between the highest occupied molecular orbital (HOMO) energy level of donor materials and the lowest unoccupied molecular orbital (LUMO) energy level of acceptor materials. J_{sc} are mainly affected by the efficiency of light absorption, exciton diffusion, charge transfer and charge collection [4]. Hence, for conjugated donor copolymer materials, the high hole transfer rate with a deep HOMO level and good absorption properties is our present struggling object.



Scheme 1. The chemical structure of D1, D2, D3 and D4