



## The role of hydrogen bonding in bulk-heterojunction (BHJ) solar cells: A review



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### ABSTRACT

Bulk-heterojunction (BHJ) solar cells have attracted tremendous attention in the recent years due to their potential to provide an earth-abundant and low cost solution to solar energy conversion. Unlike inorganic solar cells, BHJ solar cells use small molecular or polymeric light absorbers which can be delicately designed and assembled. With the aim of facilitating light absorption and improving morphology for efficient charge separation and transfer, hydrogen-bonding (H-bonding) has been employed in BHJ solar cells due to its relatively strong non-covalent interactions, highly directional and specific characteristics. The current review aims to summarize H-bonding in small molecule and polymer based donor materials as well as acceptor materials in BHJ solar cells. Emphasis will be placed on the molecular design of incorporating H-bonding in the donor and acceptor materials. The morphology optimization and power conversion efficiency (PCE) improvement in the presence of H-bonding will be the central topics of this review.

### 1. Introduction

Energy crisis and environment pollution are two of the most important issues of our time. The inevitable increase in population and the economic development that occur around the world have serious implications for the energy supply and environment protection [1]. As fossil energy sources are on the route of depletion and the fossil energy generation processes are generally polluting and harmful to the ecosystem, substitutes for these energy sources are needed to address the current issues [2]. Solar energy is extensive, inexhaustible, clean, free and renewable which can be an ideal substitute. Photovoltaics, as an efficient and direct technology to transfer solar energy into electricity, have attracted intensive research interests. Among various types of photovoltaics, BHJ organic solar cells have the potential to provide an earth-abundant and low-cost photovoltaic solution [3,4]. This technology aims to enable roll-to-roll processing techniques and allow for low-cost manufacturing [5,6]. As various absorbers can be used to create colored or transparent photovoltaic devices and the ability to be applied to flexible substrates, this technology is particularly appealing to the wearable and building-integrated photovoltaic market [7].

BHJ solar cells based on binary (or tertiary) mixtures of p-type electron donors and n-type electron acceptors fabricated through cost-effective solution-based methods is an intensively studied topic in the

academic community and the industry [8]. Advancements in the fundamental understanding of the relationship between materials and their properties and device performances have allowed BHJ solar cells to reach PCEs up to 13% [9].

Compared to traditional silicon solar cells where free charges are generated directly upon photoexcitation, splitting of excitons in BHJ organic solar cells requires to overcome a larger potential barrier (exciton binding energy > 50 meV) owing to the lower dielectric constant of the organic/polymeric medium [10]. In BHJ solar cells, this is typically achieved by mixing materials with different electron affinities and oxidation potentials, i.e. an electron donor is used in conjunction with an electron acceptor, such as a fullerene, which has molecular orbital energy states that facilitate electron transfer [11]. Because of the typical homopolar conductivity of organic materials, the transport of electrons and holes to the respective electrodes requires preferential percolation pathways of the donor and the acceptor in phase segregated domains [12]. The two components are expected to self-assemble into an interpenetrating network connecting the two electrodes. However, it is challenging to control the nanostructured morphology precisely which is critical to photovoltaic performance [13]. In order to optimize the BHJ solar cell efficiency it is therefore pivotal to finely tune the degree of blending. On one hand, a fine interpenetration assures that the size of segregated domains does not exceed two times of the exciton

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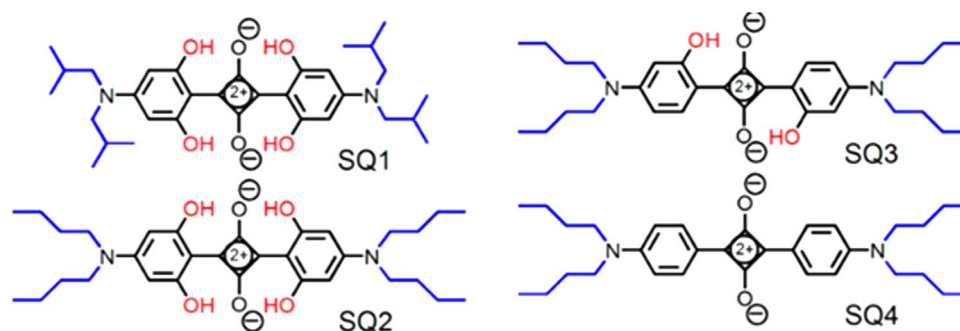


Fig. 1. Squaraine dyes locked with intramolecular H-bonding show distinct optoelectronic and self-assembly behaviors. Reprinted with permission from Ref. [33]. Copyright (2014) American Chemical Society.

diffusion length, otherwise the exciton can not reach the donor/acceptor interface and the splitting of the exciton is suppressed. On the other hand, phase separation into highly conductive crystalline domains promotes efficient charge carrier transport [14]. Molecular orientation and inter-diffusion of molecular species between phase separated domains have also been shown to affect the performances of BHJ solar cells significantly, thereby further highlighting the importance of developing means to fine-tune the self-assembly processes in donor and acceptor blends [15–19].

The H-bonding is an attractive interaction between a hydrogen atom of a molecule or a molecular fragment  $-XH$ , in which X is more electronegative than H, and an atom or a group of atoms in the same or a different molecule [20]. In the natural world, H-bonding interactions are extremely prevalent and exist in the simplest water as well as complicated DNA and proteins. H-bonding is regarded as a relatively strong, highly directional, and specific non-covalent interaction present in many organic and polymer molecules, and is notably responsible for supramolecular ordering in nature [21]. They are also the main driving force in building sophisticated artificial supramolecules and self-assembled nanostructures [24]. The bond energies of the H-bonding are typically at  $5\text{--}65\text{ kcal mol}^{-1}$  which are significantly stronger than  $\pi\text{-}\pi$  interactions ( $< 10\text{ kcal mol}^{-1}$ ) and van der Waals ( $< 5\text{ kcal mol}^{-1}$ ), but possess the flexibility and assembling ability as a non-covalent interaction [22]. The  $\pi\text{-}\pi$  interactions and van der Waals are inevitably presented in the donor and acceptor domains while the H-bonding can be selectively incorporated and delicately designed. Compared with covalent interactions, the H-bonding is much weaker but plays an important role in determining the molecular conformation and solid state packing which are important for light absorption and domain formation [23].

The role H-bonding can play in organic conducting and semi-conducting materials has been long postulated and realized by material chemists. Głowacki et al. have summarized the H-bonding in organic electronics with an emphasis on charge conductivities mediated by H-bonding [25]. However, so far there is no review about the effect of H-bonding on BHJ solar cell active layer morphology control and photovoltaic performances, even though organic solar cell is intensively studied, and a significant number of studies on H-bonded BHJ solar cell materials have emerged in literatures. This review aims to summarize the literature work of H-bonding in BHJ solar cells. Emphasis will be placed on the molecular design of incorporating H-bonding in the donor and acceptor materials. The morphology optimization and power conversion efficiency (PCE) improvement in the presence of H-bonding will be the central topics of this review.

## 2. Hydrogen bonded donor materials

For a long time, the acceptor materials are dominated by fullerene and its derivatives. The development of donor materials is much more frequently appeared in literature and acts as a primary driving force for

achieving high PCEs. As a consequence, H-bonding is widely studied in the donor materials. Chemists designed and synthesized various types of H-bonded donor materials in the aim of control molecular conformation and film morphology through self-assembly. Applications of such systems in BHJ solar cells exhibited improved performances and enhanced our understanding in the structure-property relationship of the materials in BHJ solar cells.

### 2.1. Intramolecular H-bonded donor materials

To improve PCEs of BHJ solar cells, first and foremost, the molecular structure of donor molecules should be carefully designed by considering their close relationship with the photovoltaic parameters, including short-circuit current density ( $J_{sc}$ ), open-circuit voltage ( $V_{oc}$ ) and fill factor ( $FF$ ) [26,27]. Broadening the absorption bandwidth of BHJ solar cells by controlling the molecular conformation of the donor materials is an attractive means of resolving the narrow absorption of organic semiconductors. The intramolecular interactions play important roles in the material solid-state organization. An effective approach to planarize a small molecular or polymer chain (without losing its solution processability) is to create a noncovalent attractive interaction between neighboring moieties via intramolecular interactions [28–32]. Hydrogen bonds, dipole–dipole interactions, and intramolecular O–S interactions have been demonstrated to be effective for minimizing torsional angles within small molecule and polymer backbones [25]. On increasing the coplanarity of a polymer chain with close solid-state  $\pi\text{-}\pi$  stacking, both polaron and exciton delocalization and their transport characteristics can be improved.

Hido et al. purposely tuned the side chains and number of hydroxyl (OH) groups in a series of squaraine (SQ) dyes, to investigate the effect of structural variations on the material properties as well as the performance of these dyes as donor materials in BHJ solar cells (Fig. 1) [33]. Their results showed that the OH groups deepened the highest occupied molecular orbital (HOMO) of the donor and thus enhanced the  $V_{oc}$ , whereas the linear chain improved the charge transport properties in the BHJ solar cell active layers. Both the side chain and the number of OH groups can influence the aggregation behavior of these SQs in solid-state films. This phenomenon is most likely due to the strong intermolecular coupling and H-bonding interactions between  $-O^-$  and the  $-OH$ , resulting in the formation of a planar molecular structure and a head-to-tail packing mode. Thus SQ1 and SQ2 which contain four  $-OH$  group displayed better BHJ solar cell performance than SQ3 and SQ4 which contain only two or no  $-OH$  groups. Solution-processed BHJ solar cell using SQ1 as donor and [6,6]-phenyl-C71-butyric acid methyl ester (PC<sub>71</sub>BM) as acceptor showed PCEs up to 4.0%.

Kim and Woo et al. developed a series of dialkoxyphenylene-benzothiadiazole containing semicrystalline low band gap polymers with non-covalent conformational locking to enhance chain planarity, intermolecular ordering and thermal stability without losing solution processability (Fig. 2) [34]. The polymers formed well-distributed

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