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Theoretical investigation on the white-light emission from a single-polymer system with simultaneous blue and orange emission (Part II)

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ABSTRACT

We report here a theoretical investigation of the white-light emission from a single-polymer system with simultaneous blue (polyfluorene as a blue host) and orange (2,1,3-benzothiadiazole(BTD)-based derivative as an orange dopant) emission. With use of quantum-chemical approaches, our studies are focused on the variation in electronic and optical properties as a function of the chemical composition of the backbone in BTD-based derivatives. Furthermore, the results show that the electronic and optical properties of designed BTD-based derivatives can be tuned by the introduction of suitable electron-donating groups on terminal *N*,*N*-disubstituted amino groups, implying good candidates as orange dopants in WPLEDs with polyfluorene as a blue-light-emitting host. In addition, low reorganization energy values of holes or narrow differences between hole and electron transportations within the framework of the charge hopping model suggest designed BTD-based derivatives to be good hole transport or ambipolar transport materials in organic light-emitting diodes. It is also found that the designed BTD-based derivatives containing fluorene-based unit exhibit higher stability.

1. Introduction

White organic light-emitting devices based on polymers (WPLEDs) have received great attention because they can be easily fabricated using wet processes, including the spin casting, screen-printing, and ink-jet printing techniques, which are expected to be lower in cost in mass production, especially in the production of large-area panel displays [1–8]. Among these devices, white electroluminescence (EL) from a single-polymer is extremely desirable because it can offer several distinct advantages, such as low cost, simple fabrication processes, and ease of scaling up, without any problems associated with phase separation of components. In this field, Wang et al. propose a novel strategy to realize the white EL with simultaneous blue, green, and red emission from a single-polymer [4]. Similarly, they also propose a strategy to develop the white emission from a single-polymer by incorporating a small amount of orange emission component into a blue-light-emitting polymer [5]. For example, they succeed in realizing highly efficient white EL with simultaneous blue and orange emission from a single-polymer, in which a small amount of orange-light-emissive 1,8-naphthalimide derivatives or 2,1,3-benzothiadiazole (BTD) derivatives are incorporated into the main chain of a blue-light-emitting polyfluorene.

A number of studies demonstrate the interplay between theory and experiment, which is capable of providing useful insights to the understanding of the molecular electronic structure of the ground and excited state as well as the nature of absorption and photoluminescence [9,10]. In our previous report [10], we selected a single-polymer

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electroluminescent system containing two individual emission species (polyfluorene, $(PF)_n$, as a blue host and a BTD-based derivative, $(OMC\text{-}CH_3)_m$, as an orange dopant) as model compounds (shown in Fig. 1a) to explore their experimentally observed electronic and spectroscopic behaviors in depth on the basis of the quantum-chemical calculations. Our computational results have provided a reasonable interpretation of the experimental findings.

With the aim to design novel orange dopants, in this continuous investigation, some asymmetric derivatives were designed as the backbone of orange dopants by introducing cyclopentadithiophene (CPDT) or fluorene (F) (shown in Fig. 1b) to BTD-based derivatives. Where special attention is devoted to the variation in properties as a function of the chemical composition of the backbone in 4,7-bis(4-(*N*,*N*-diphenylamino)phenyl)-2,1-3-benzothiadiazole [11] (OMC, shown in Fig. 1b), toward better understanding of the structure–property relationships and thus the acquiring knowledge on how to develop new orange dopants in WPLEDs with $(PF)_n$ as a blue-light-emitting host. Fluorene-containing materials are the most intensively investigated π-conjugated materials in many fields [12] because of their excellent electrical and optical properties, good thermal and chemical stability, and the ease of processing. Similarly, thiophene-based π-conjugated polymers have received a great deal of attention because of potential applications in organic light-emitting diodes (OLEDs) that take advantage of their excellent chemical, thermal, and photochemical stabilities as well as ease of structural tuning to adjust the electronic and morphological properties [13]. Therefore, it is of practical significance to extend our previous work to a comprehensive theoretical investigation on these two types of BTD-based derivatives in which one of triphenylamine (TPA) units of OMC is replaced with CPDT or F unit (Fig. 1b). In addition, increasing attention has been attracted to the introduction of heteroatoms into the traditional π-conjugated organic system composed of carbon and hydrogen [12c,14] because the significant orbital interaction between heteroatom and the organic π-conjugated part is a highly effective way to produce desired electronic structures. Here, the carbon atom at position 8 or 9 (labeled as X, shown in Fig. 1b) in CPDT or F is substituted with boron, silicon, nitrogen, oxygen, sulfur, and selenium, which permit us to check the influence of these heteroatoms on the electronic and optical properties of explored derivatives. We also check the electronic and optical properties of designed CPDT-/F-substituted derivatives by adding

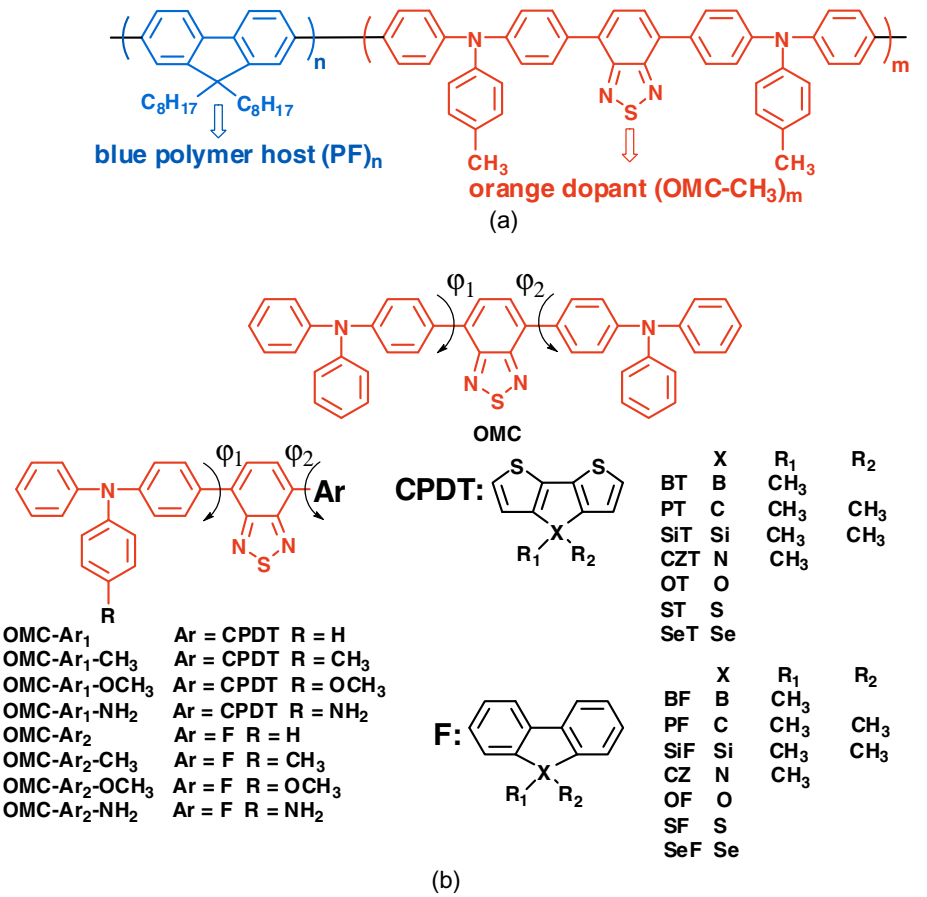

Fig. 1. (a) The chemical structure of the model polymer –$(PF)_n$–$(OMC\text{-}CH_3)_m$–. (b) Chemical structures of the investigated BTD-based derivatives (OMC and its derivatives).