



# Structure-property relationship of phosphine oxide based thermally activated delayed fluorescence molecules: First-principles study

Xiangpeng Kong, Lei Cai, Jianzhong Fan, Lili Lin\*

Shandong Province Key Laboratory of Medical Physics and Image Processing Technology, Institute of Materials and Clean Energy, School of Physics and Electronics, Shandong Normal University, 250014, Jinan, China



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## ABSTRACT

Three phosphine oxide (P=O) based blue TADF emitters with weak acceptors and strong donors (WASD) were reported recently by Xu' group [*Chem. Mater.* **2016**, *28*, 5667], which provides a new way for the design of blue TADF emitters. To reveal the relationship between the geometric structures and the photophysical properties, twelve P=O based molecules are theoretically studied based on first-principles calculations. It is found that the numbers of donor groups have weak effect on the emission wavelengths since more molecular orbitals are involved in the excitation except the highest occupied molecular orbital and the lowest unoccupied molecular orbital. With the increase of the numbers of donor groups, the energy gap between the first singlet excited state (S1) and the first triplet excited state (T1) becomes narrower. However, the electron donating ability of more donors becomes a little weaker. In addition, the investigation of the types of donor groups on the S1-T1 energy gap indicates that the 9,9-dimethyl-9,10-dihydroacridine (DMAC) group is better than other kinds of donors to narrow the S1-T1 energy gap. In addition, the meta-position is also proven less efficient than the para-position to obtain a small S1-T1 energy gap. Our theoretical study will be helpful to the design of P=O based TADF emitters.

## 1. Introduction

Thermally activated delayed fluorescence (TADF) molecules have become the research focus of both experimental and theoretical workers [1–6], since the external quantum efficiency of the pure organic light-emitting diodes (OLEDs) exceeded the limit of conventional fluorescent OLEDs [7–10]. Until now, most of TADF molecules reported are composed of donors (D) and acceptors (A) [11,12]. For blue TADF molecules, weak donors and strong acceptors are usually used. In general, two kinds of acceptors are adopted. One is the conjugated (benzotrifluoride, pyridine, triazine, thioxanthone, etc.) [13,14], and the other is the insulating acceptors (carbonyl, sulfone, etc.) [15,16]. For the conjugated acceptors, bathochromic shift is invariably found in emission spectra when intramolecular conjugation is extended or the enhancement of the overlap between donors and acceptors [17]. Recently, Xu' group reversed the strategy and adopted strong donors and weak acceptor (phosphine oxide, P=O group) to obtain true-blue TADF emitters [17–20]. It was the first reported P=O based weak acceptor and strong donor (WASD)-based TADF emitter. It was also found that the emission color is preserved when the conjugation extension is added and the external quantum efficiency reached up to 16.3%. This verified

the effectiveness of the WASD strategy in developing high-performance blue TADF emitters. However, we note that only a few kinds of P=O based TADF emitters have been reported until now [21,22], and most of P=O based molecules are designed as host materials in OLEDs [23–27]. Consequently, detail investigation of the photophysical properties of P=O based TADF molecules are quite necessary.

In this paper, the excited properties of the three P=O based TADF emitters (Group1 shown in Fig. 1) are studied theoretically. To further obtain the structure-property relationship, other P=O based molecules are theoretically designed. In these molecules, 9,9-dimethyl-9,10-dihydroacridine (DMAC) and 3,7-dimethoxy-10H-phenoxazine (DMOPXZ) are adopted as donor groups (Group 2 and Group3 shown in Fig. 1). The influence of the donor groups on the excited properties of P=O based molecules are investigated. In addition, the numbers of donor groups or the conjugation extension on the molecular properties are also studied based on three kinds of P=O based molecules. At last, the donor groups are changed from the para-position to the meta-position (Group 4 shown in Fig. 1) [28], which will help us to make out of the relationship between the relative positions and the excited properties. All these results will help one better understand the influence of the structures on the excited properties of P=O based molecules, and

\* Corresponding author.

E-mail address: [linll@sdu.edu.cn](mailto:linll@sdu.edu.cn) (L. Lin).

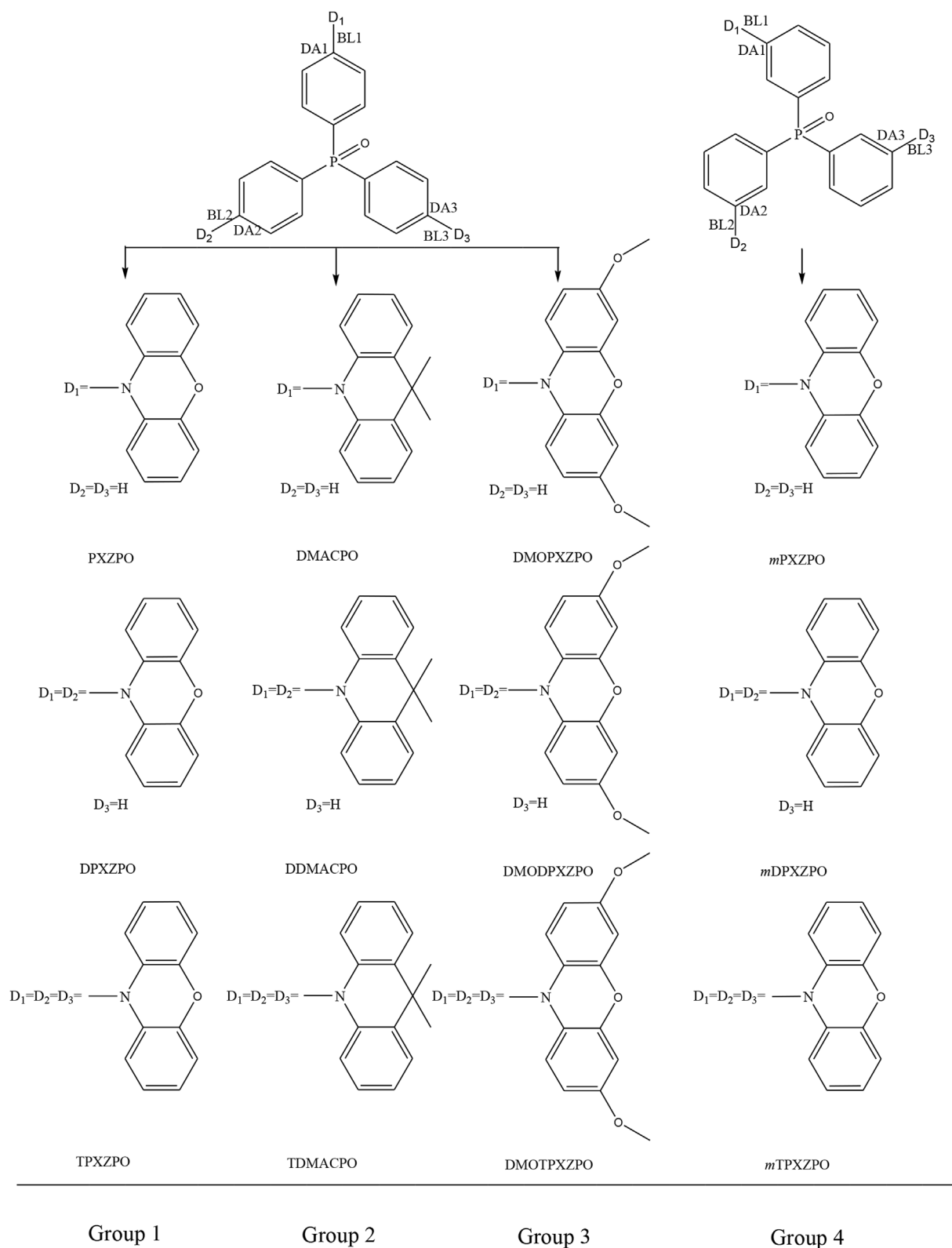


Fig. 1. Geometric structures of P=O based molecules studied..

will promote the design of high-performance TADF molecules.

## 2. Theoretical methods

In this study, the geometry and the electronic structures are investigated using the density functional theory (DFT) at the B3LYP/6-

31G level. Correct calculation of the energy gap between the first singlet excited state (S1) and the first triplet excited state (T1) theoretically is a challenging work, and several methods have been proposed [19,29,30]. Considering the computation correction and cost, the optimal HF (OHF) method which has been widely used to predict the S1-T1 energy gap is adopted here [19,31,32]. In this method, different

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