2-phenylfuro[2,3-b]quinoxaline-triphenylamine based emitter: photophysical property and application for TADF-sensitized fluorecence OLEDs

Xinye Wang†, Yixiang Li†, Yuan Wu, Ke Qin, Defei Xu, Dongdong Wang*, Huili Ma*, Shuya Ning, and Zhaoxin Wu

Electronic Supplementary Information

Contents

Section 1:Computational details

The quantum mechanics/molecular mechanics (QM/MM) theory with two-layer ONIOM method was implemented to deal with the electronic structures in crystal, where the central molecule is chosen as the active QM part and set as the high layer, while the surrounding ones are chosen as the MM part and defined as the low layer (Figure S1). The universal force field (UFF) was used for the MM part, and the molecules of MM part were frozen during the QM/MM geometry optimizations. The electronic embedding is adopted in QM/MM calculations by incorporating the partial charges of the MM region into the quantum mechanical Hamiltonian. Molecular geometry optimizations were performed for the ground (S0) and excited (S1) states at the level of (TD)B3LYP/def2-SVP. Based on the S1-geometry, the excitation energies and natural transition orbitals (NTO) of the low-lying excited states were evaluated at the TD-B3LYP/def2-SVP level. All calculations were performed by using Gaussian 09 program1. The spin-orbit coupling matrix elements of singlet and triplet excited states were carried out based on the first-order Douglas−Kroll−Hess-like spin−orbit operator derived from the exact two-component (X2C) Hamiltonian by using Beijing Density Function (BDF) program.[2-5]

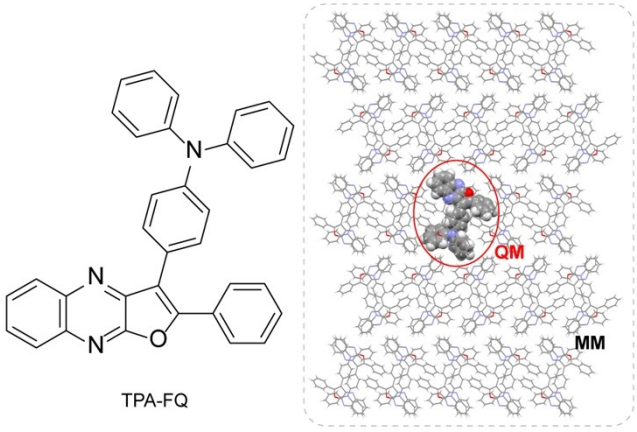

Figure. Setup of the QM/MM model, taking **TPA-FQ** as an example.

Section 2 Figures

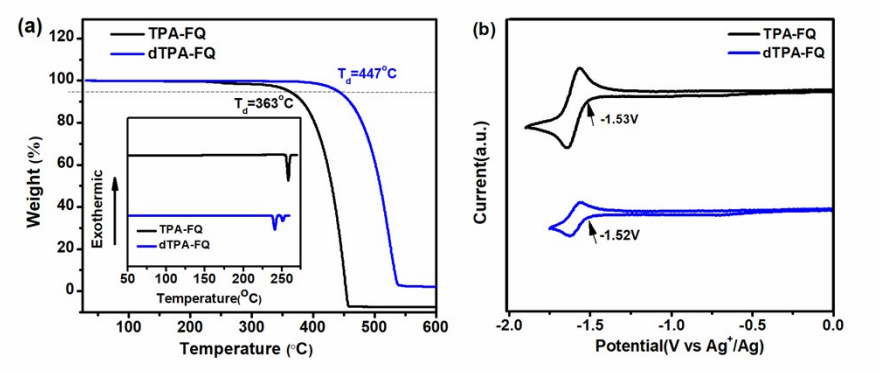

Figure S1 (a) TGA and DSC (inset) curves, and (b) CV curves of the TPA-FQ and dTPA-FQ.

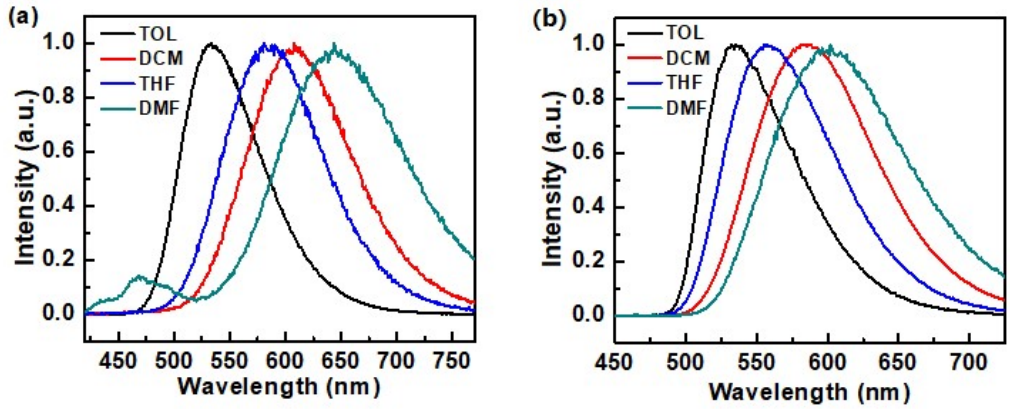

Figure S2 The PL spectra for TPA-FQ (a) and dTPA-FQ(b) in different solvents.

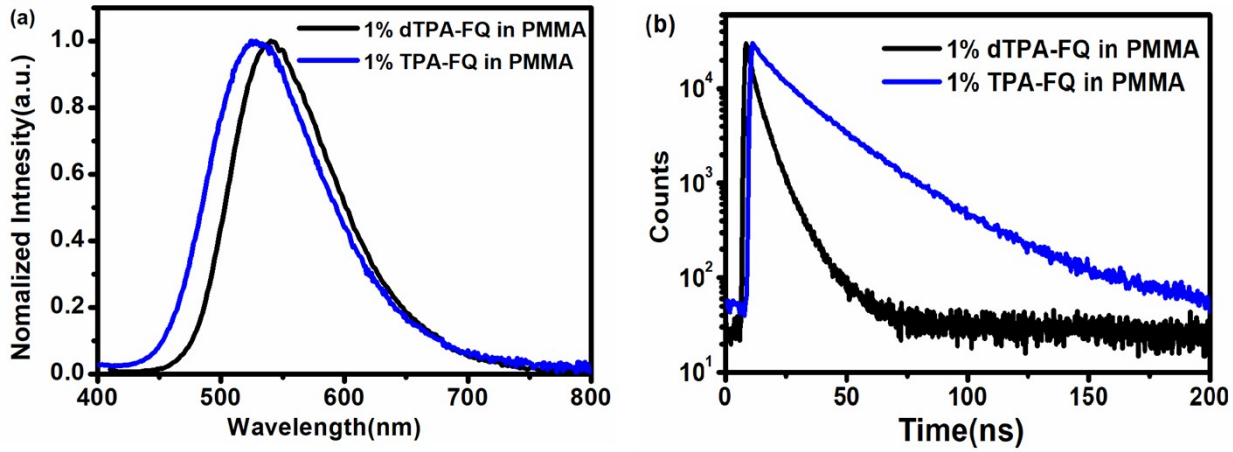

Figure S3 The PL (a) and transient PL (b) spectra of 1% TPA-FQ and 1% dTPA-FQ doped in PMMA, respectively.

Section 3: NMR spectra

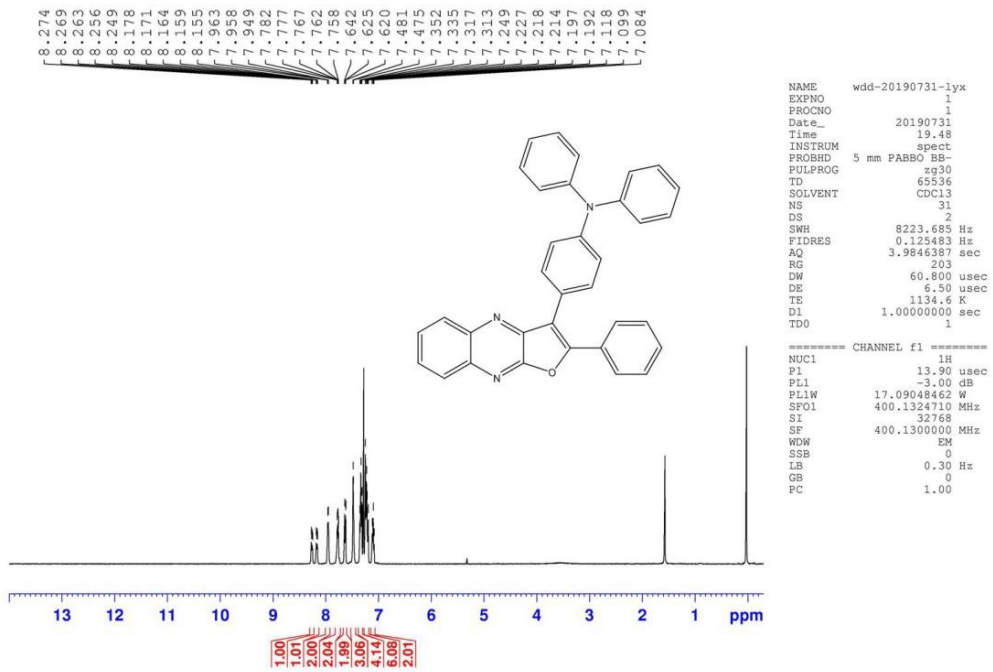

Figure S4 ^{1}H NMR spectrum of TPA-FQ

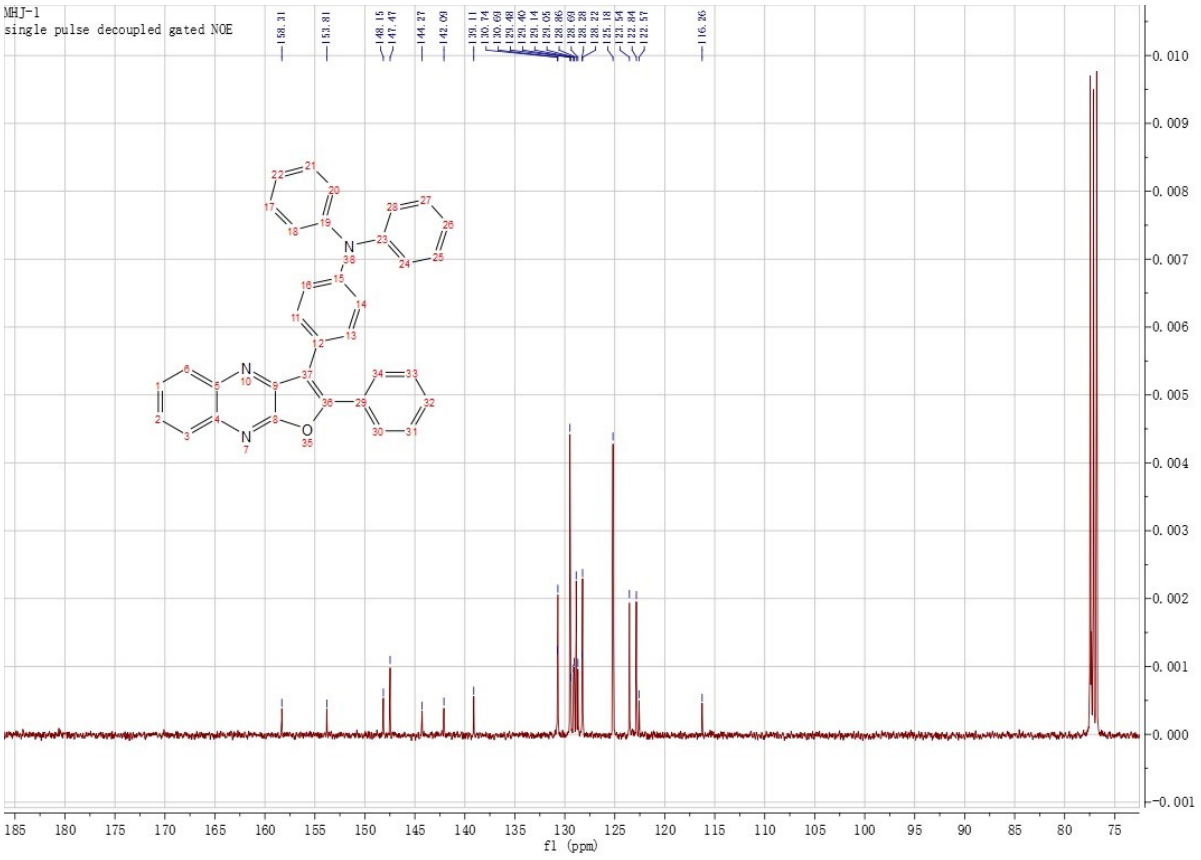

Figure S5 ^{13}CNMR spectrum of TPA-FQ

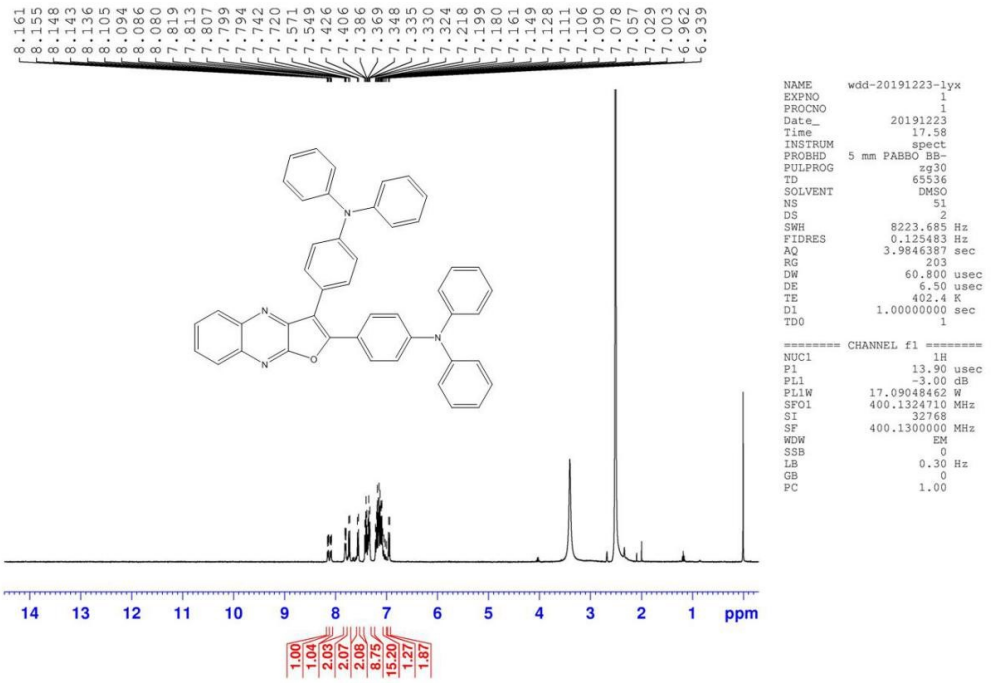

Figure S6 ^{1}H NMR spectrum of dTPA-FQ

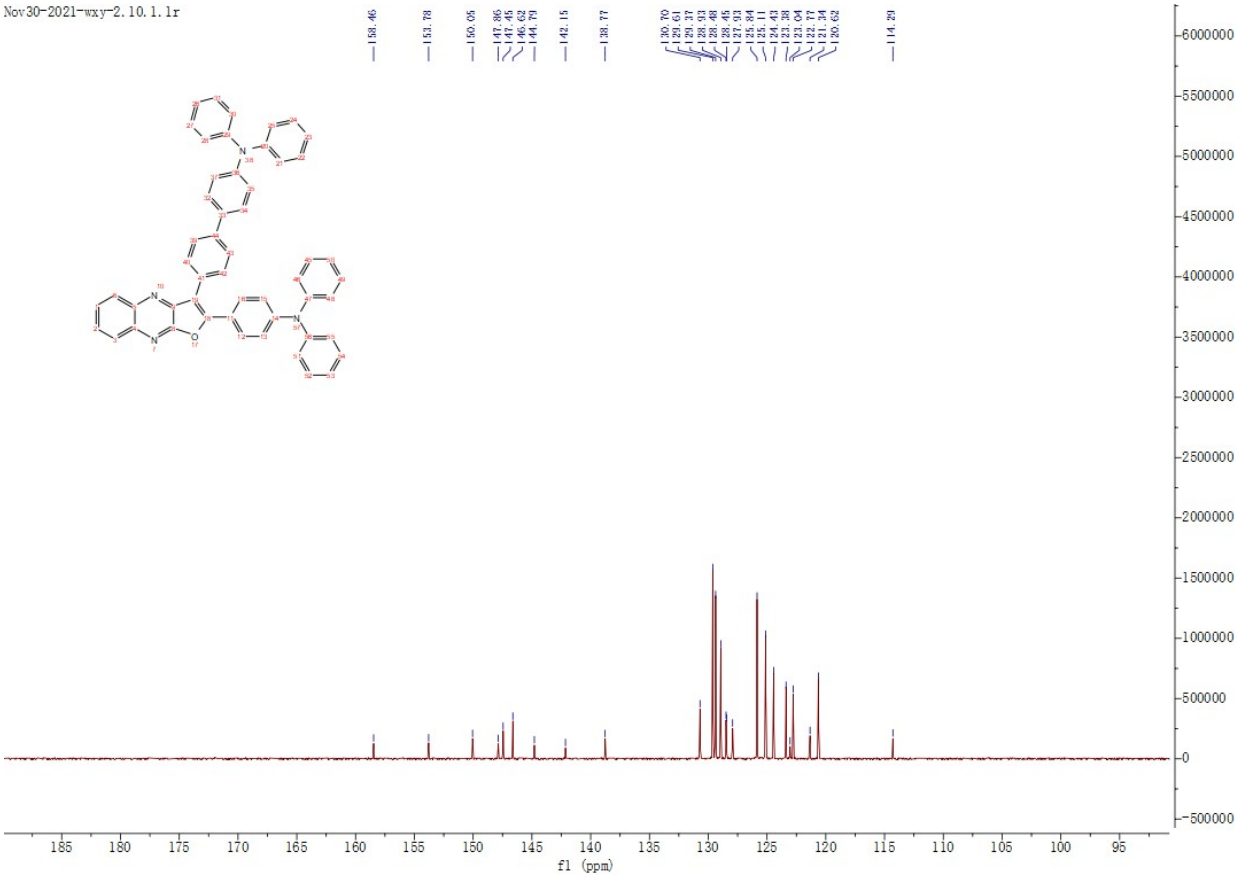

Figure S7 ^{13}C NMR spectrum of dTPA-FQ

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