Supporting Information

The Nature of the Lowest Singlet and Triplet Excited States of Organic Thermally Activated Delayed Fluorescence Emitters: A Self-Consistent Quantum Mechanics/Embedded Charge Study

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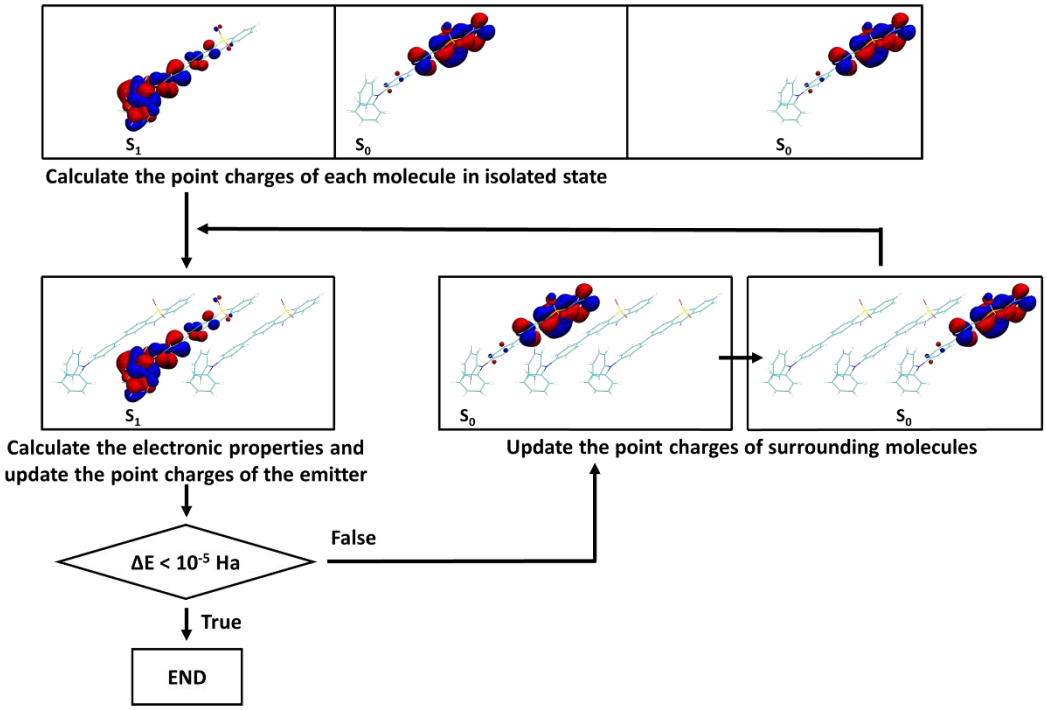

Figure S1. Schematic description of the self-consistent QM/EC approach.

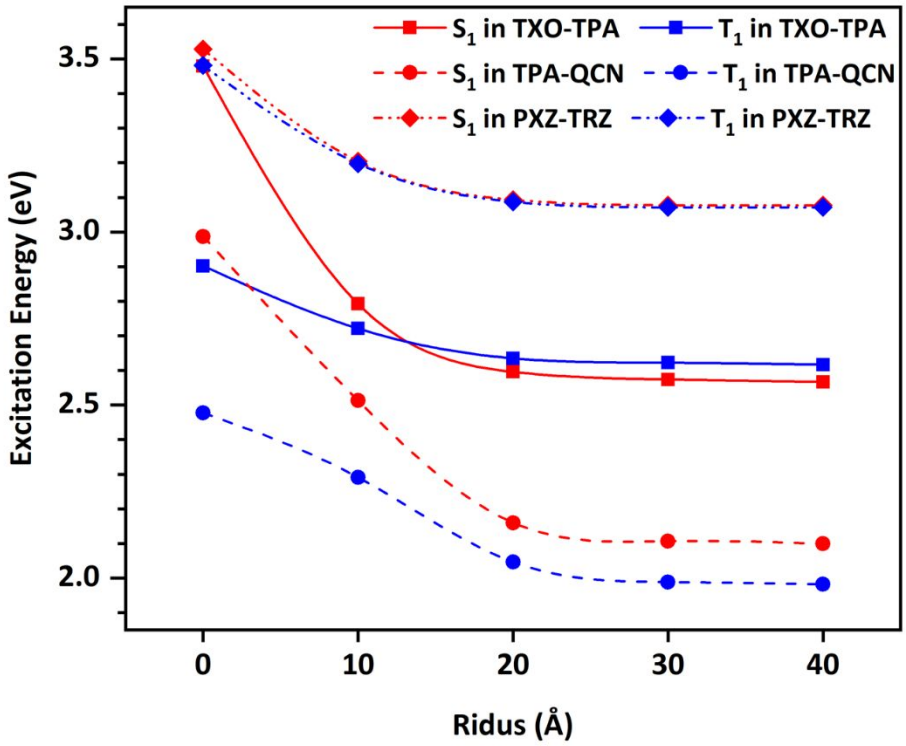

Figure S2. Dependence of excitation energies on the radius of polarizable region.

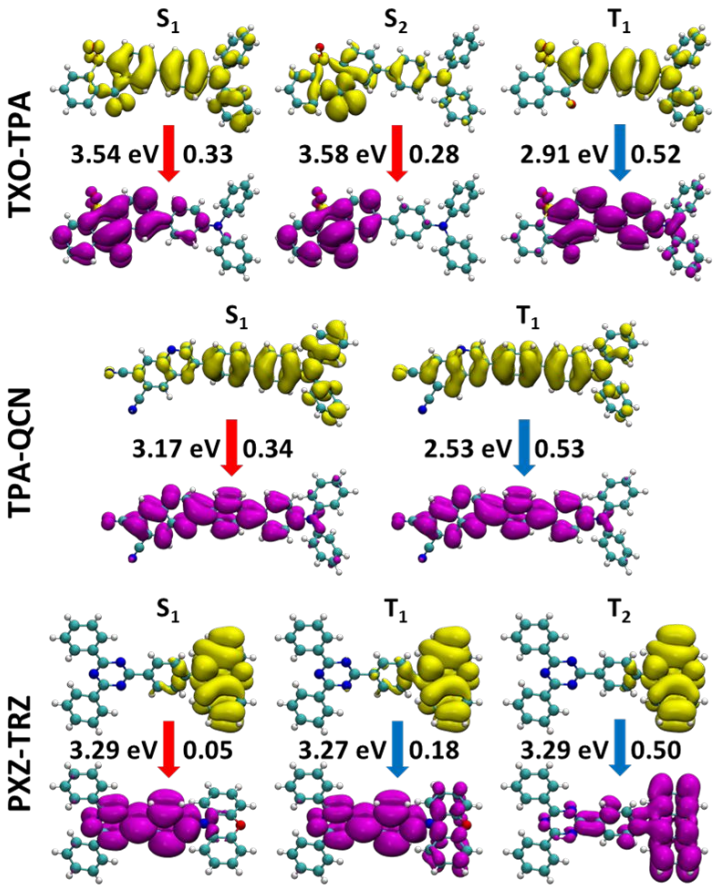

Figure S3. Hole (in yellow) and electron (in purple) density distribution for the lowest singlet and triplet excited states calculated at the TDA ωb97X*/def2-SVP level in gas phase. Excitation energies and overlap between hole and electron wave functions are also indicated.

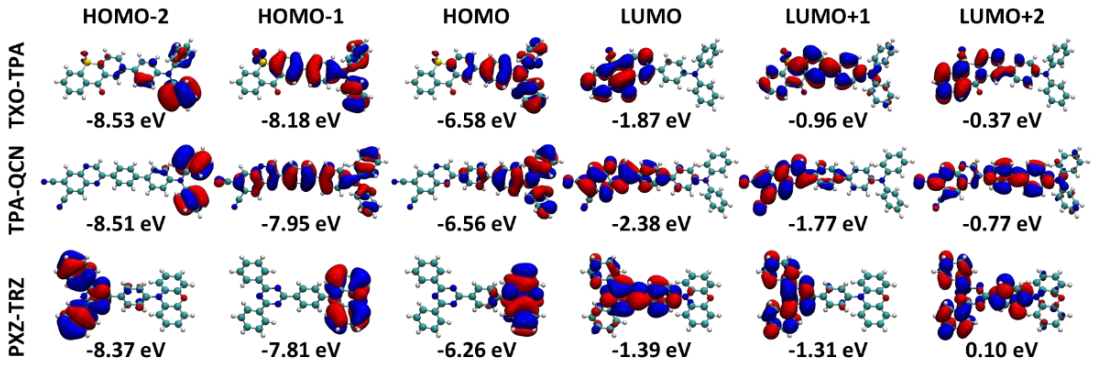

Figure S4. The frontier occupied and unoccupied orbitals and energy levels in gas phase.

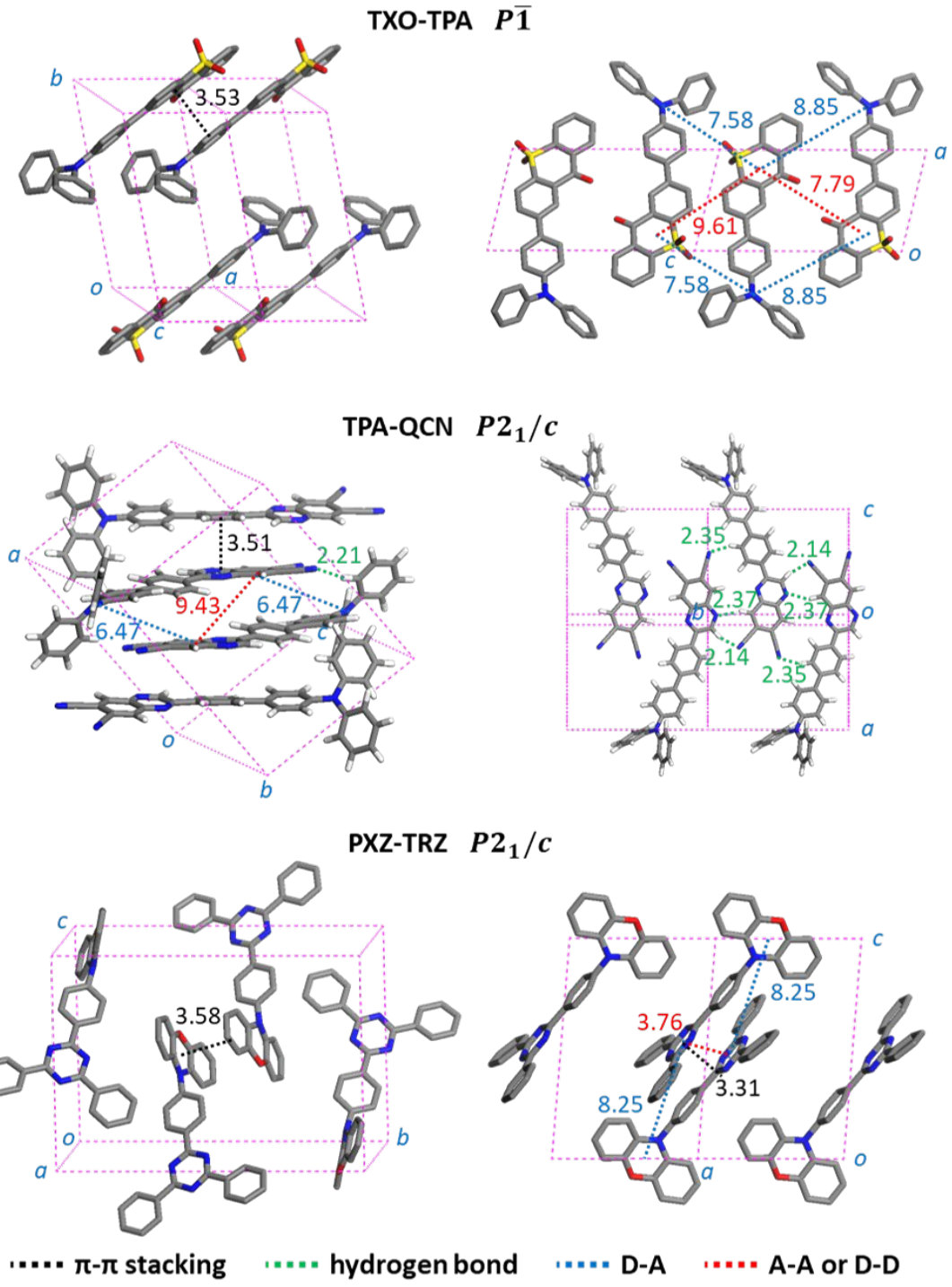

Figure S5. Diagrams of crystal packing structures of TXO-TPA (a = 6.83 Å, b = 13.11 Å, c = 14.09 Å, α = 107.68°, β = 100.92°, and γ = 96.47°), TPA-QCN (a = 16.05 Å, b = 13.22 Å, c = 12.02 Å, $\alpha = \gamma$ = 90.00°, and β = 97.86°) and PXZ-TRZ (a = 9.04 Å, b = 19.71 Å, c = 13.73 Å, $\alpha = \gamma$ = 90.00°, and β = 94.52°).

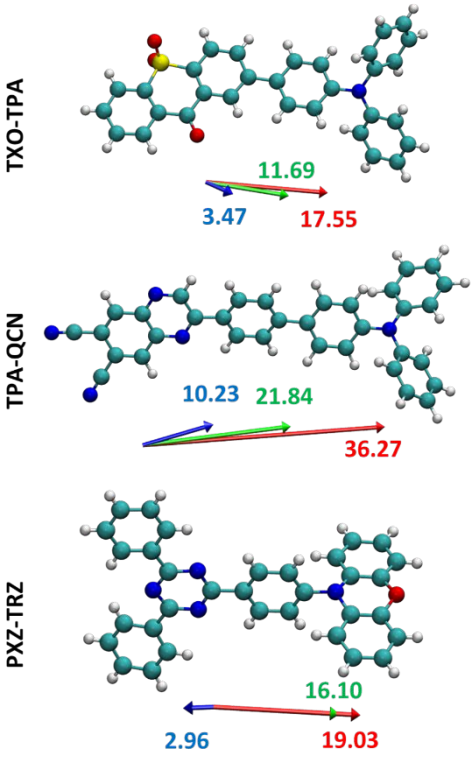

Figure S6. Dipole moments (in Debye) of the ground state (in blue), the S_1 state (or the S_2 state for TXO-TPA, in red), and the T_1 state (in green) in gas phase.