Supporting Information for

The role of intermolecular interaction in regulating the thermally activated delayed fluorescence and charge transfer properties: a theoretical perspective

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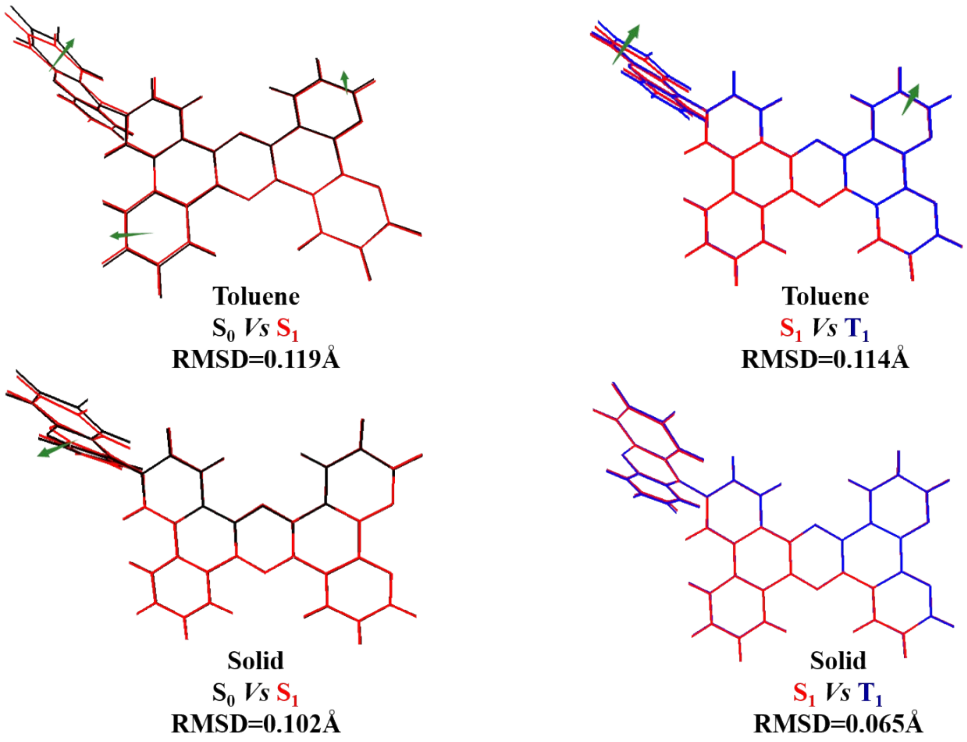

Figure S1. Geometry comparisons for BPPZ-PXZ between S_0 (black), S_1 (red) and T_1 (blue) in toluene and solid phase respectively.

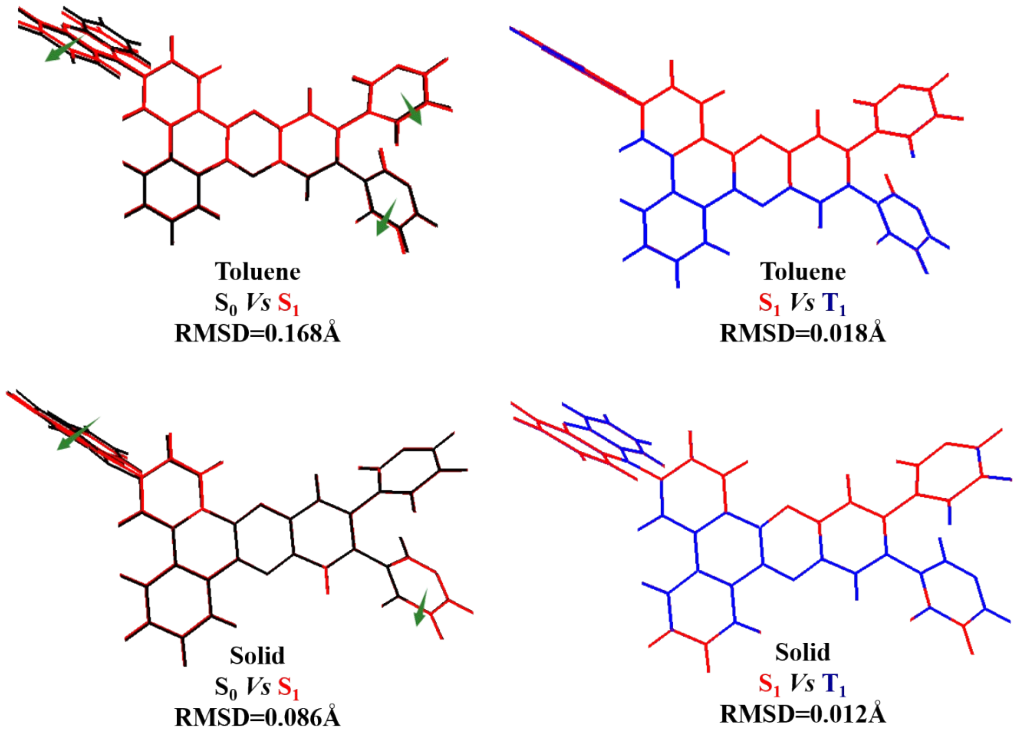

Figure S2. Geometry comparisons for mDPBPZ-PXZ between S_0 (black), S_1 (red) and T_1 (blue) in toluene and solid phase respectively.

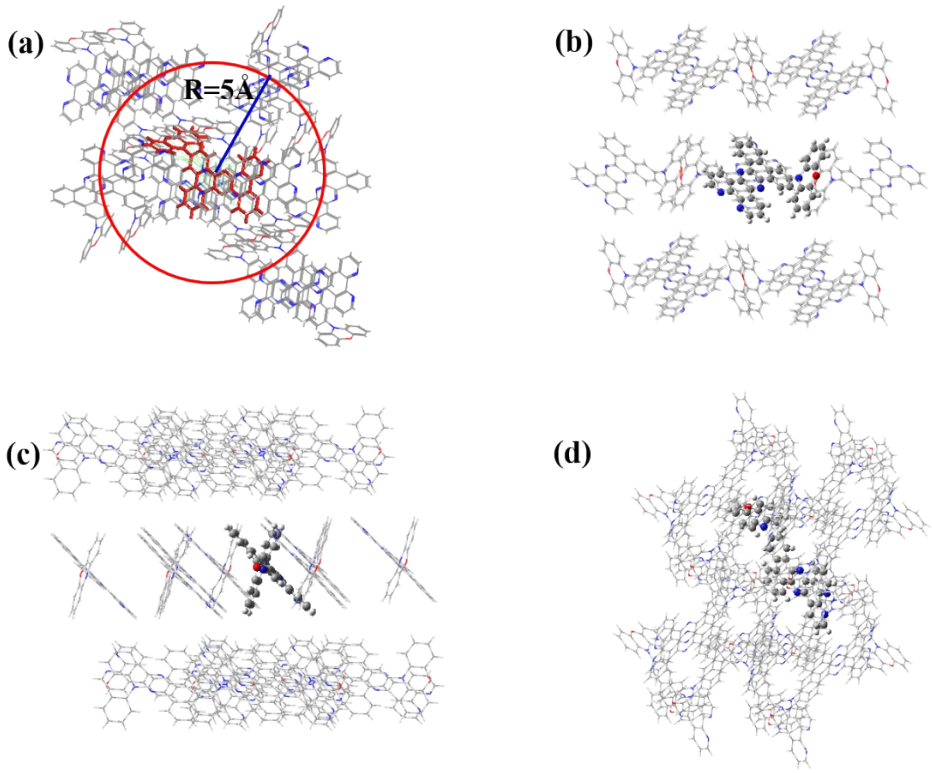

Figure S3. The sphere with a radius of 5Å for the dimer selection of BPPZ-PXZ (a). View for the QM/MM model from X-axis (b), Y-axis (c) and Z-axis (d).

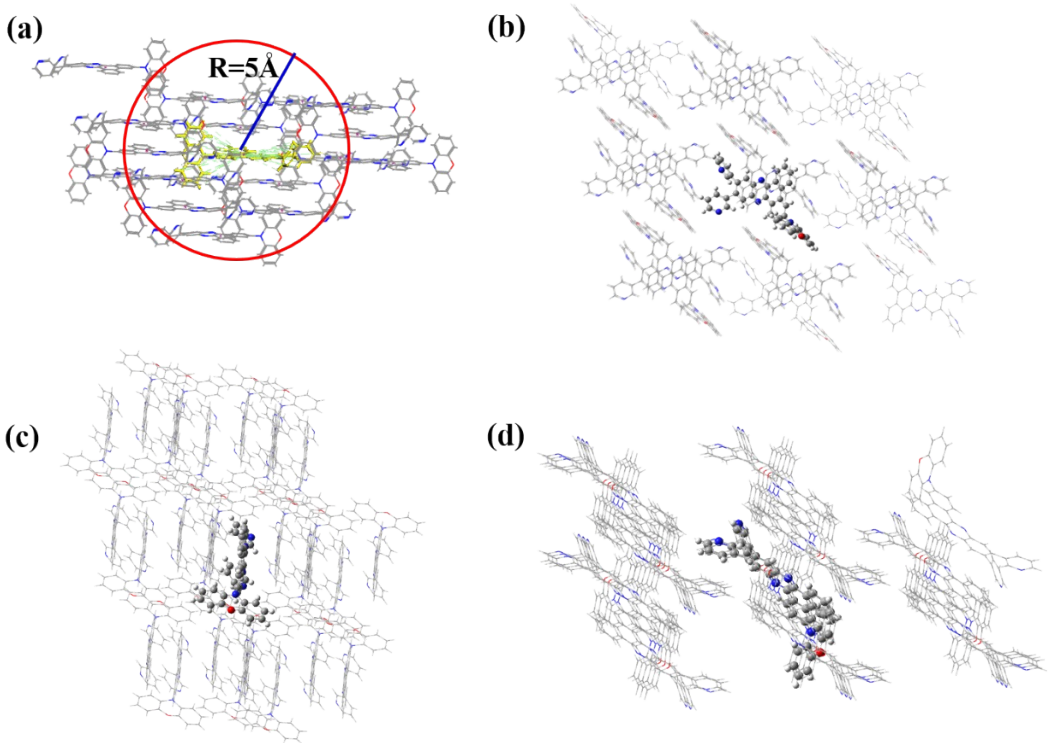

Figure S4. The sphere with a radius of 5Å for the dimer selection of mDPBPZ-PXZ (a). View for the QM/MM model from X-axis (b), Y-axis (c) and Z-axis (d).

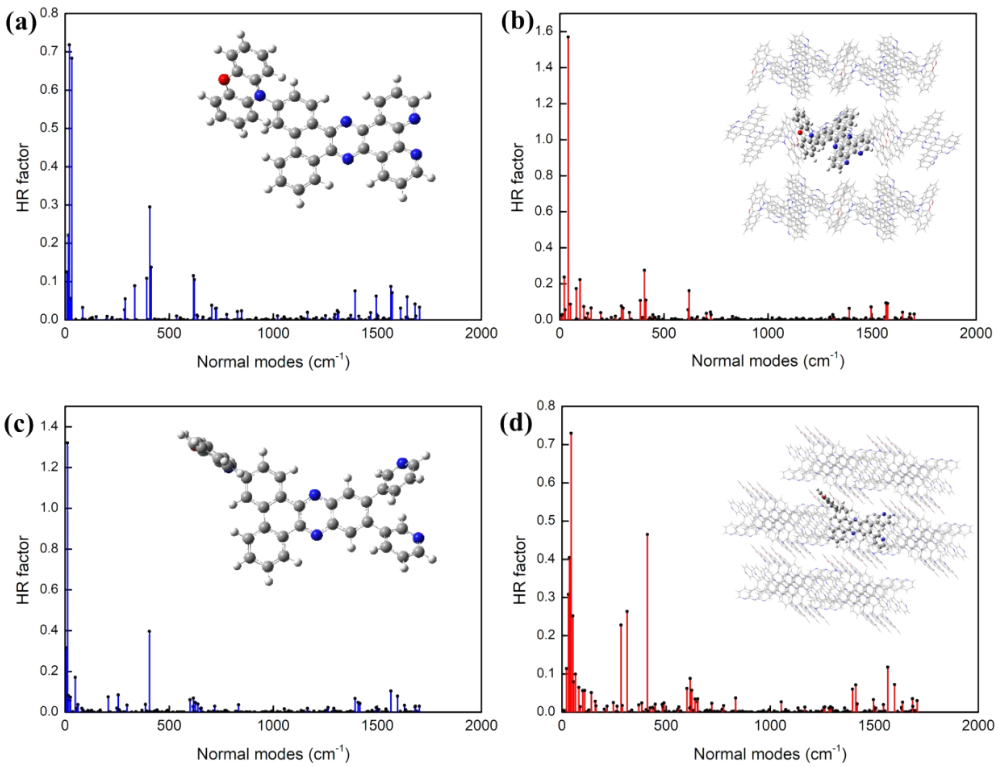

Figure S5. Calculated HR factor versus the normal mode frequencies for BPPZ-PXZ and mDPBPZ-PXZ in toluene (a, c) and the solid phase (b, d) respectively.