Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting Information for

Towards boosting exciton lifetime and efficiency of near-infrared aggregation induced emitter with hybridized local and charge transfer excited state: a multiscale study

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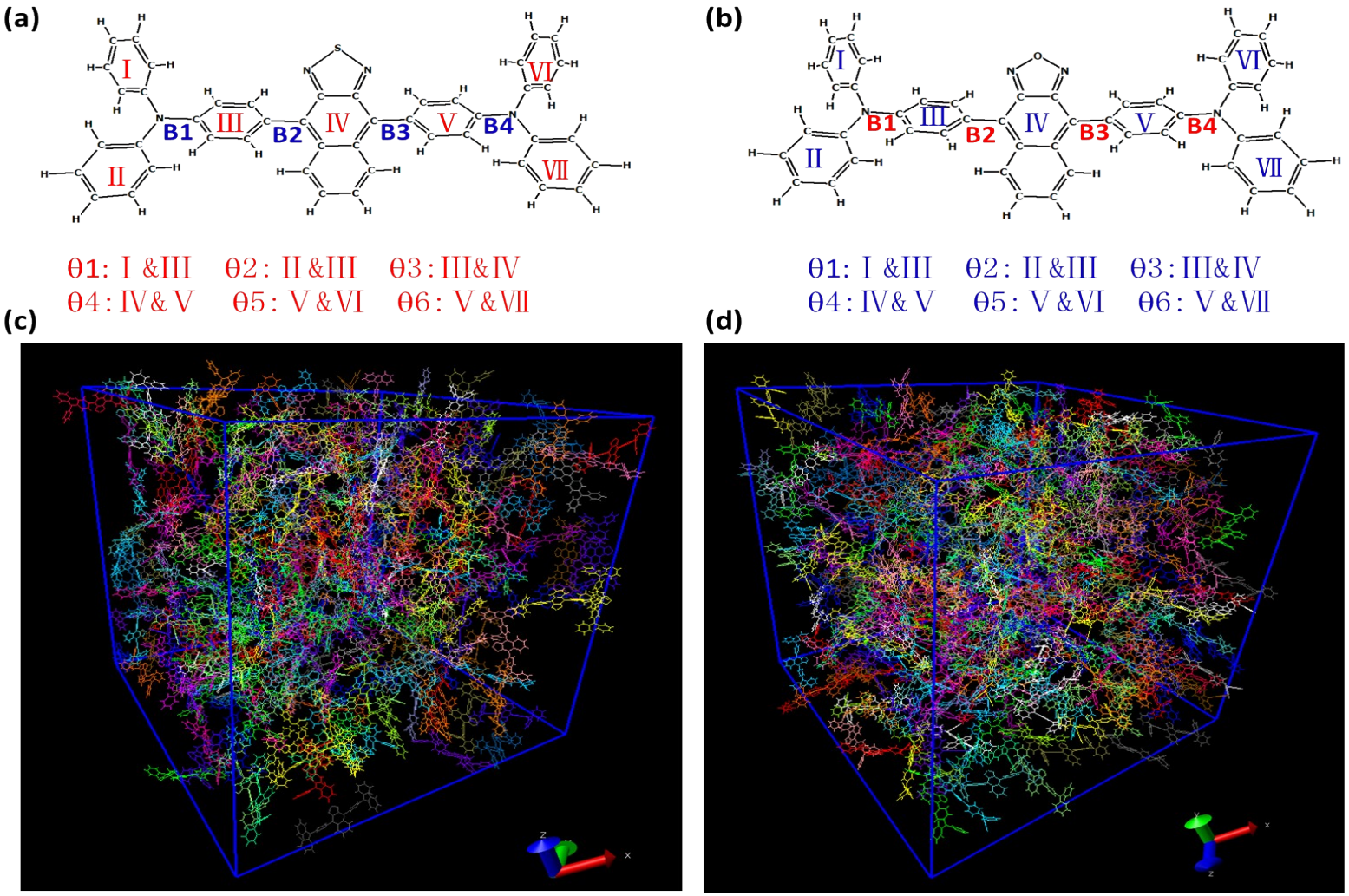

Fig. S1 The interesting dihedral angles and bond lengths of NZ2TPA (a) and NO2TPA (b). Film structure of NZ2TPA (c) and NO2TPA (d).

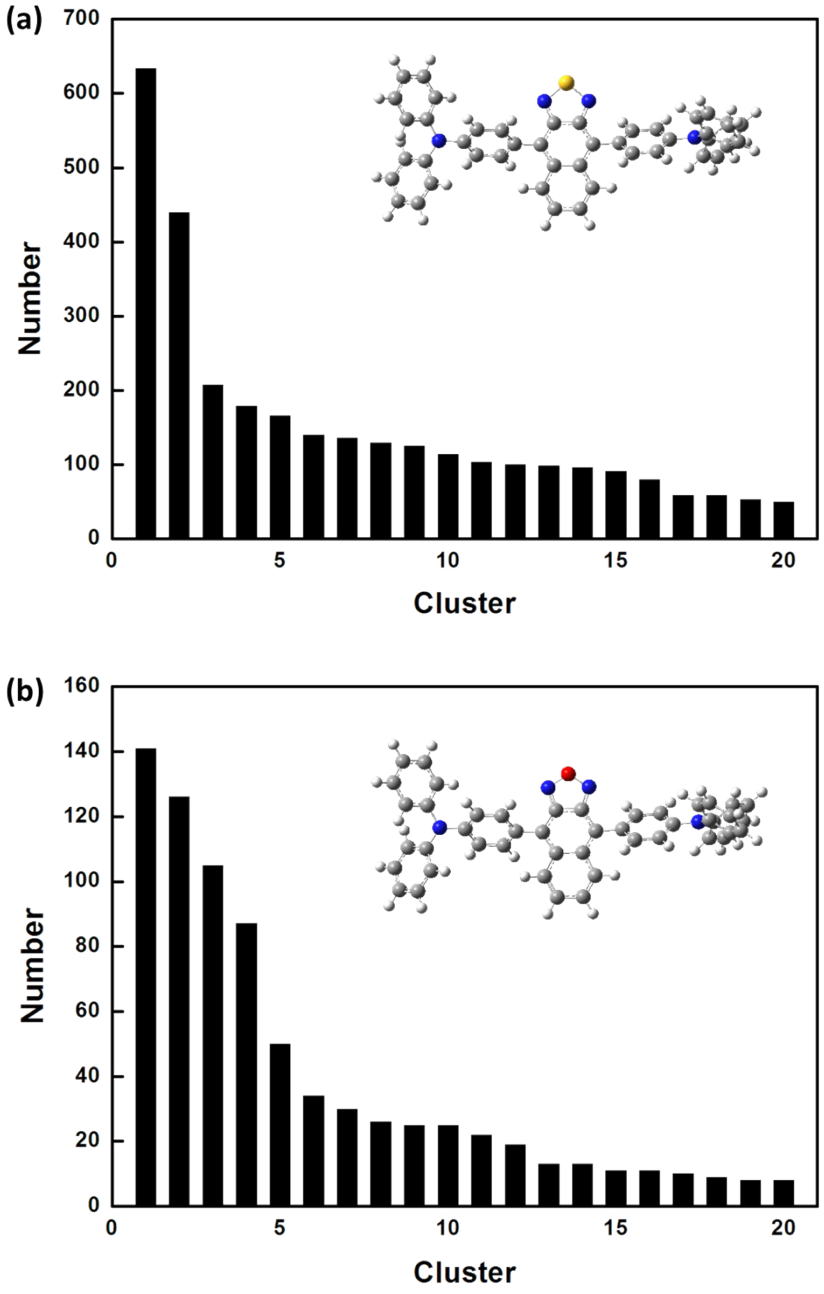

Fig. S2 Cluster analysis for the last 5ns of the simulation process for NZ2TPA (a) and NO2TPA (b).

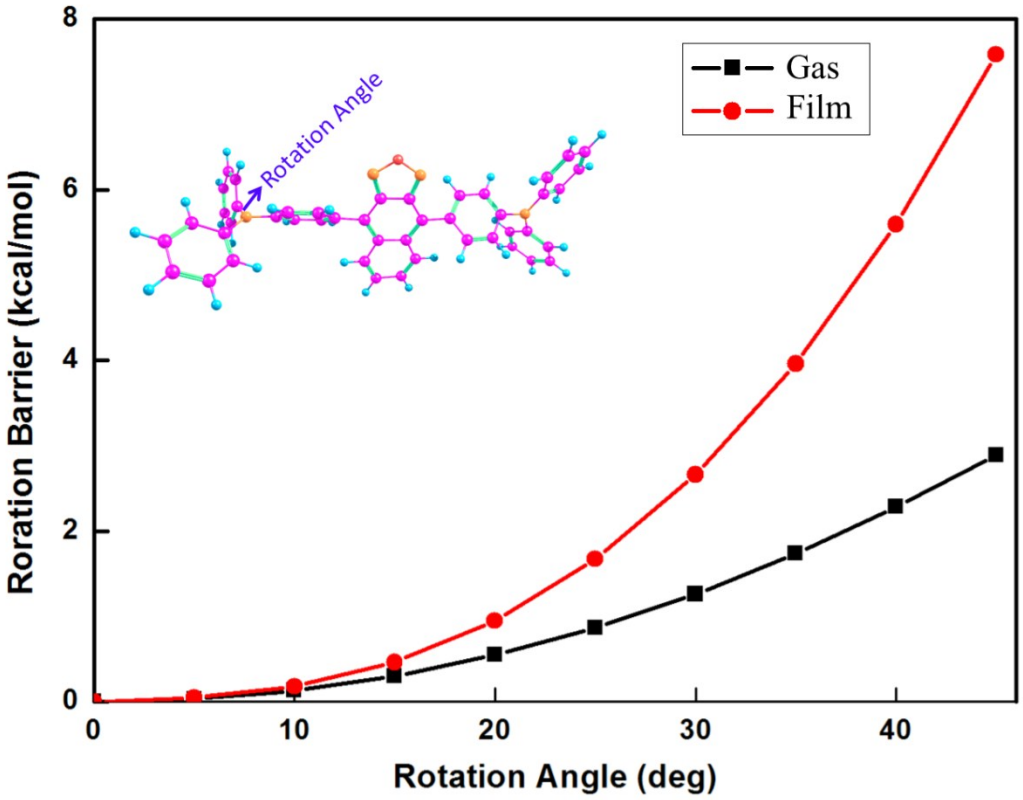

Fig. S3 Rotational energy barriers (kcal/mol) for NO2TPA in gas phase (black line) and film (red line) respectively.

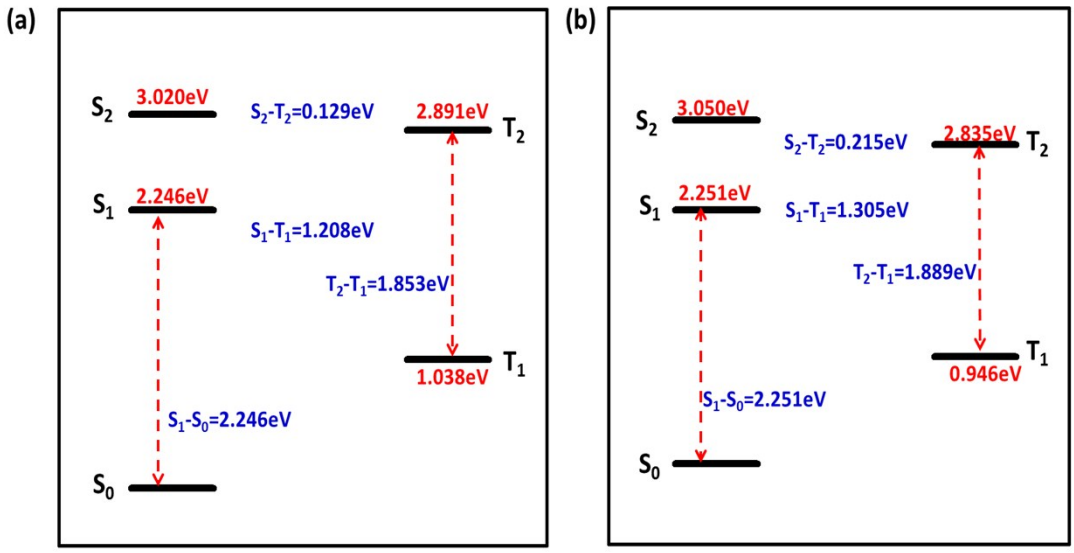

Fig. S4 Adiabatic excitation energies for NZ2TPA (a) and NO2TPA (b) in gas phase respectively.

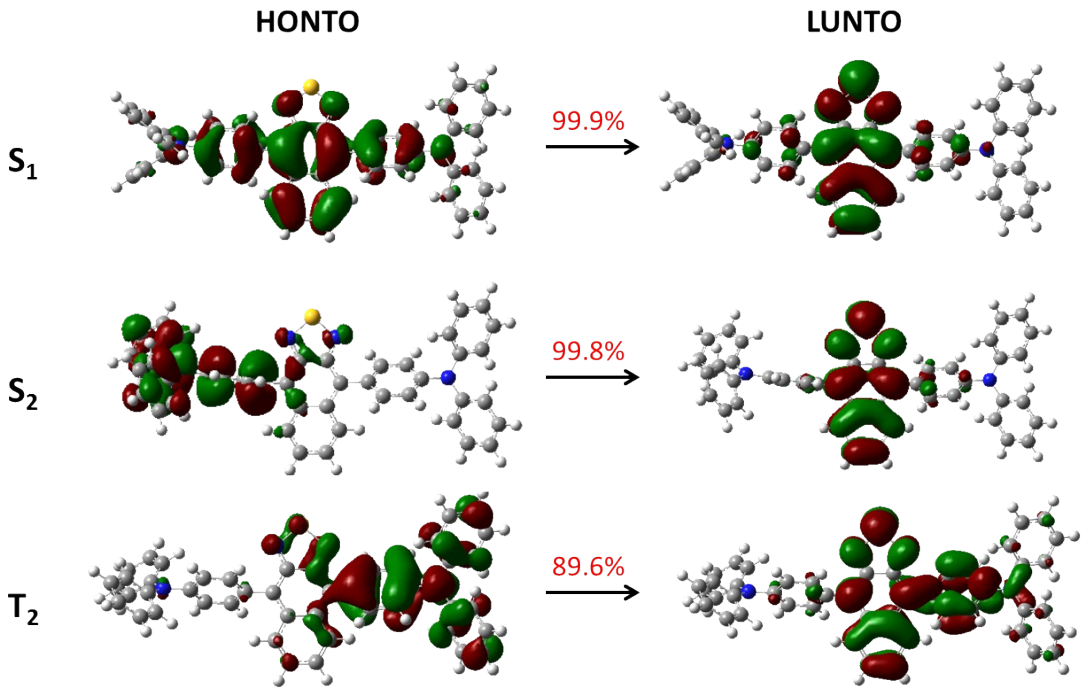

Fig. S5 Transition characteristics for selected singlet and triplet excited states for NZ2TPA in gas phase (isovalue=0.02).

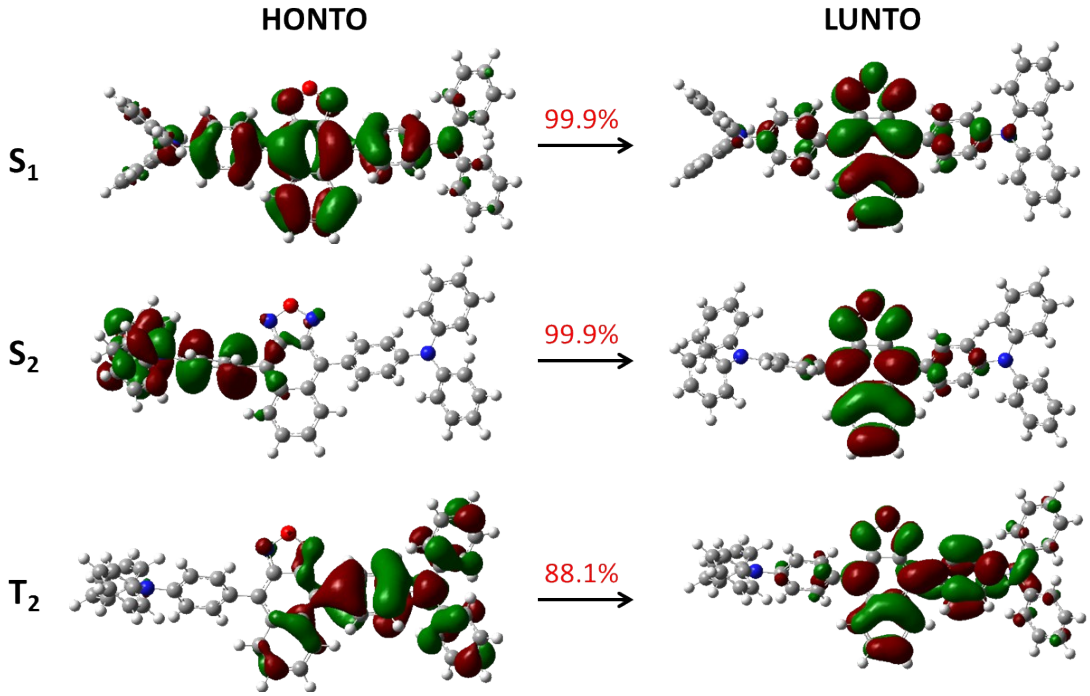

Fig. S6 Transition characteristics for selected singlet and triplet excited states for NO2TPA in gas phase (isovalue=0.02).

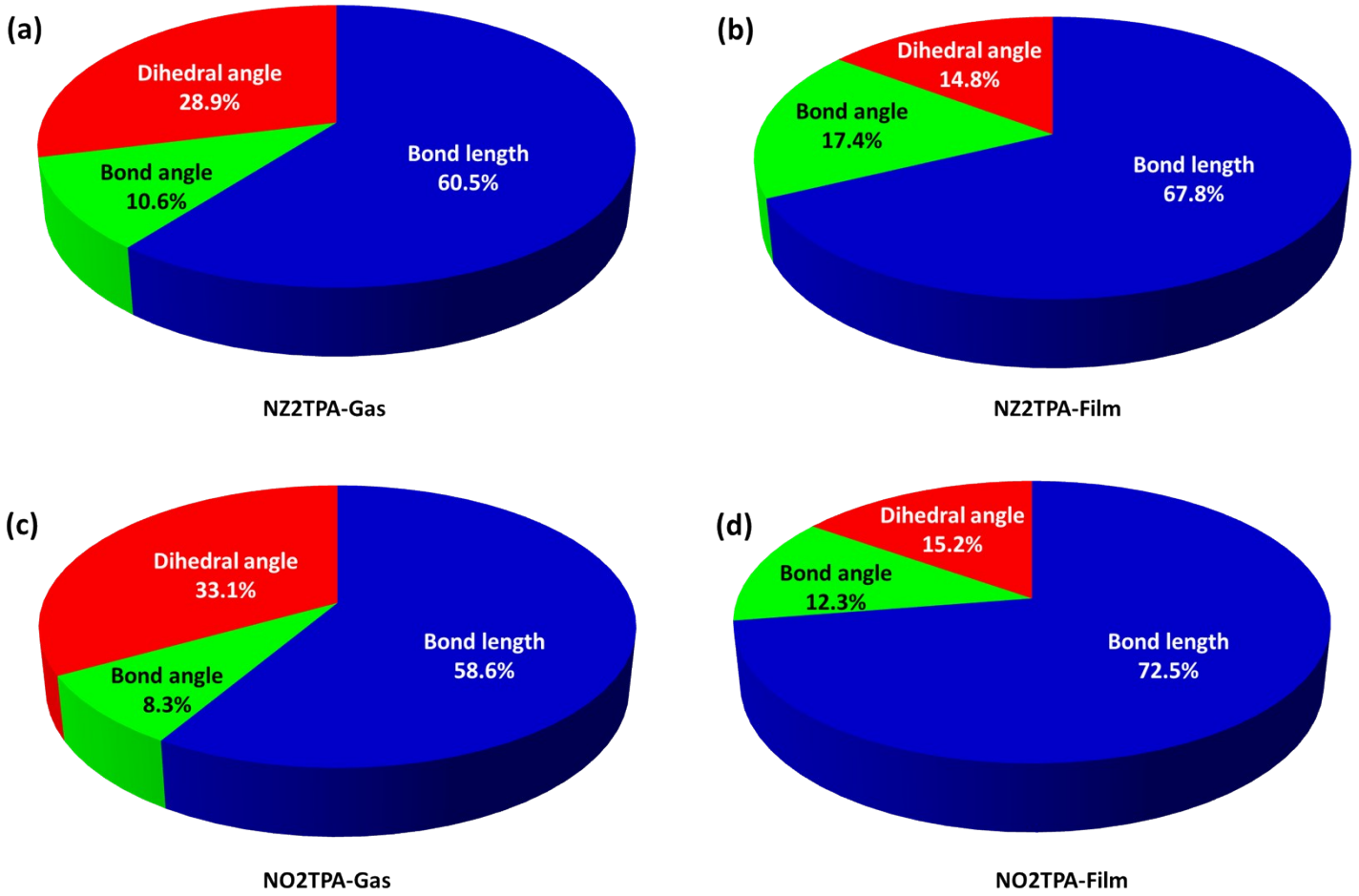

Fig. S7 Contribution ratios to the reorganization energy from bond length (blue), bond angle (green) and dihedral angle (red) of NZ2TPA (a, b) and NO2TPA (c, d) in gas phase and film respectively.

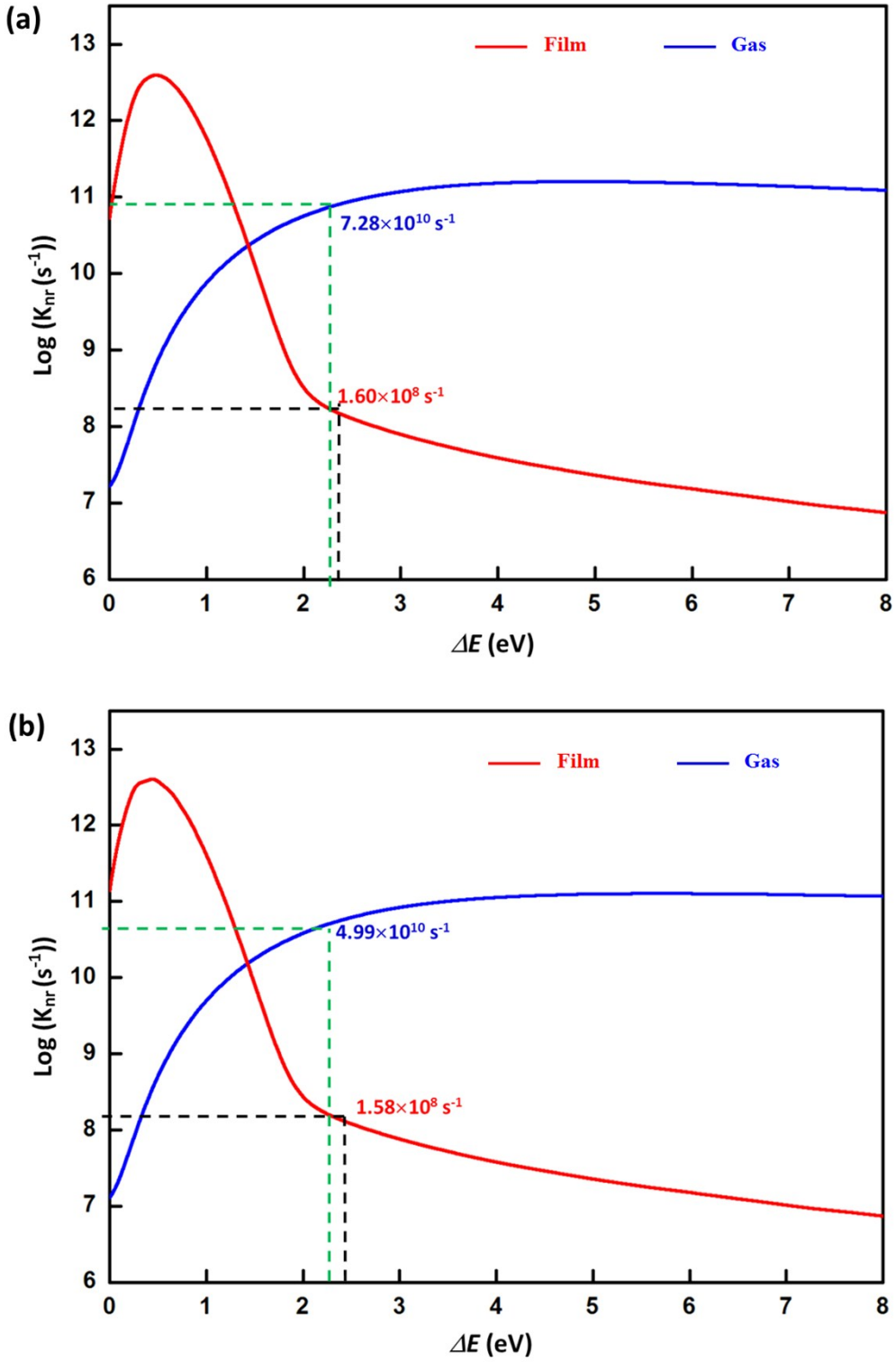

Fig. S8 Non-radiative decay rate k_{nr} from S_1 to S_0 versus the adiabatic energy gap ΔE for NZ2TPA (a) and NO2TPA (b) in gas phase (blue) and film (red) respectively.

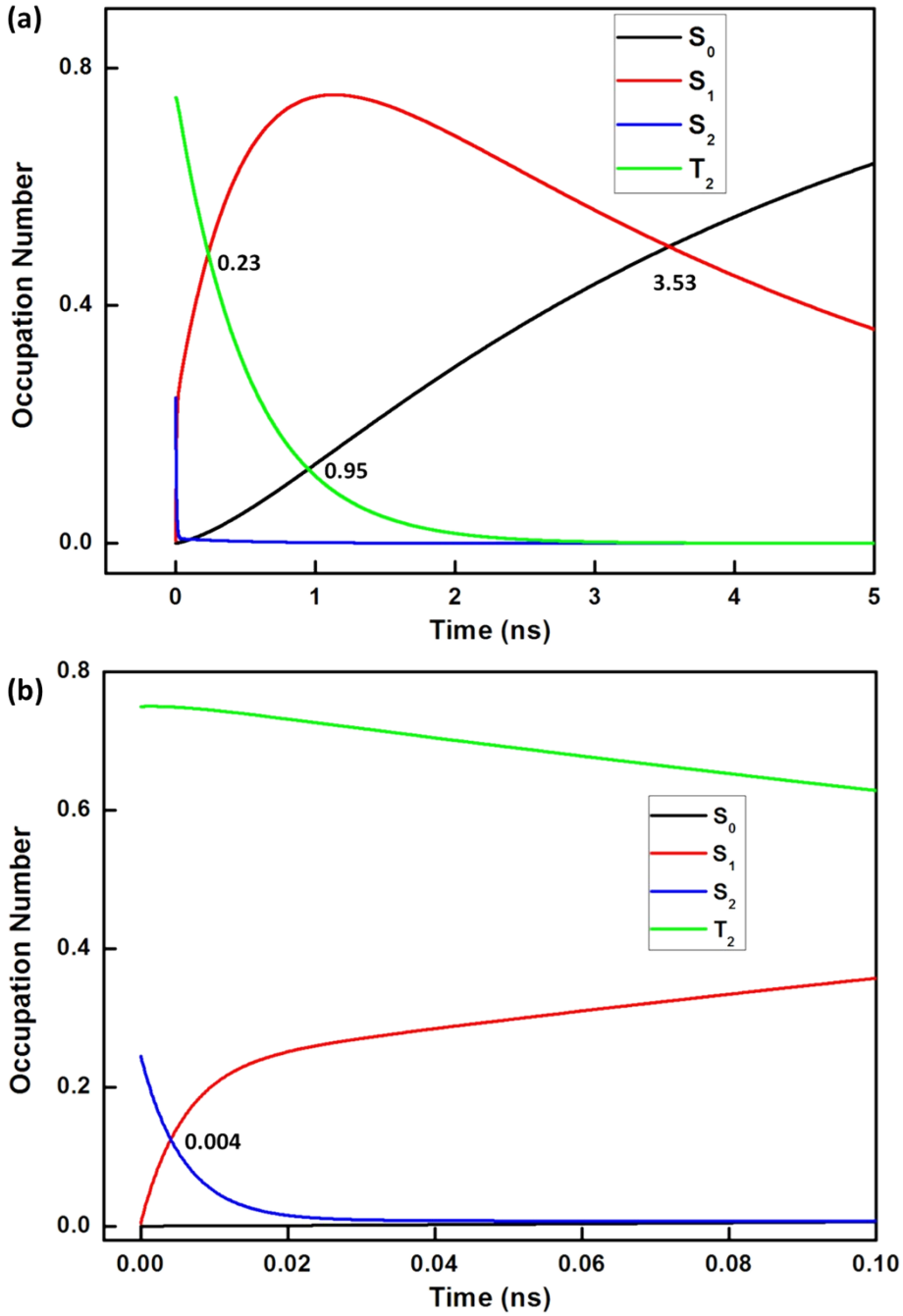

Fig. S9 Exciton evolution process of 0~5 ns (a) and 0~0.1 ns (b) for NZ2TPA in film.

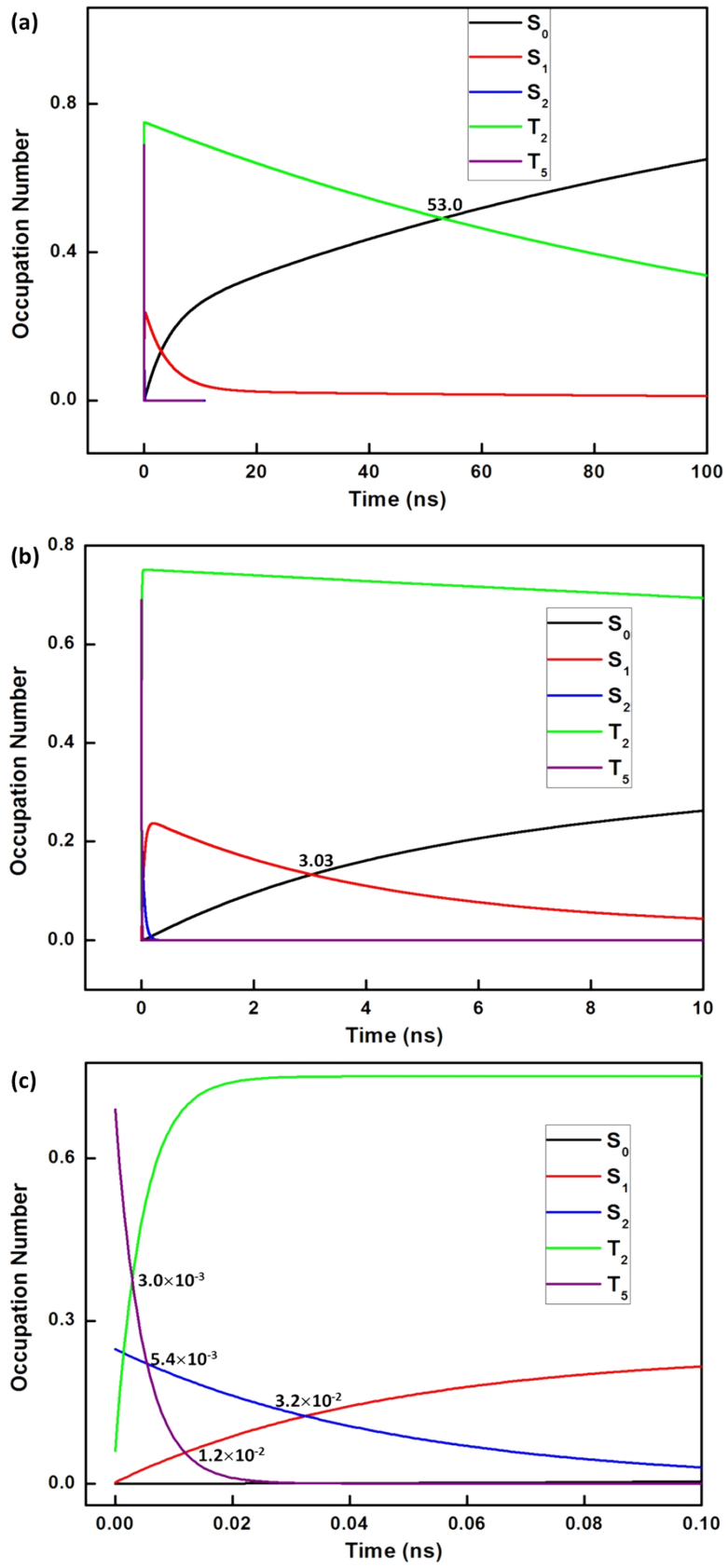

Fig. S10 Exciton evolution process of 0~100 ns (a), 0~10 ns (b) and 0~0.1 ns for NO2TPA in film.

Table S1. Calculated charge transfer (CT) and local excitation (LE) characters (in %) for selected singlet and triplet excited states of NZ2TPA and NO2TPA in gas phase.

	NZ2TPA-gas		**NO2TPA-gas**	
	LE	**CT**	**LE**	**CT**
S_1	76%	24%	80%	20%
S_2	16%	84%	15%	85%
T_2	62%	38%	65%	35%