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

Supporting Information for

Excited State Property of Non-doped Thermally Activated Delayed Fluorescence Emitters with Aggregation-Induced Emission: A QM/MM study

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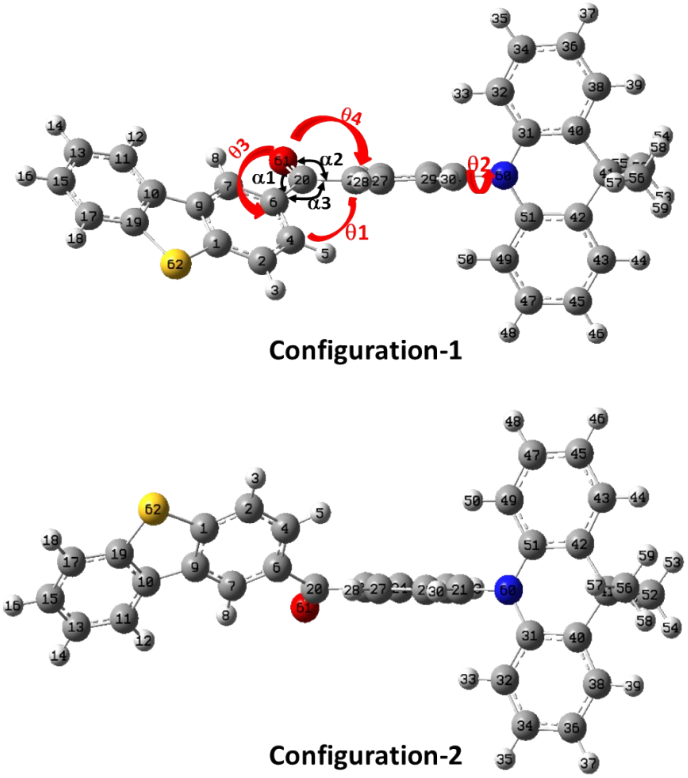


Figure S1. Two ground state configurations of DBT-BZ-DMAC.

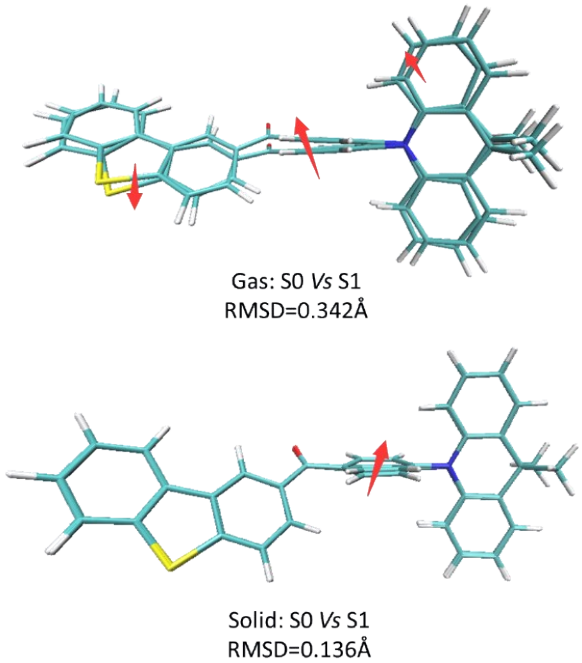
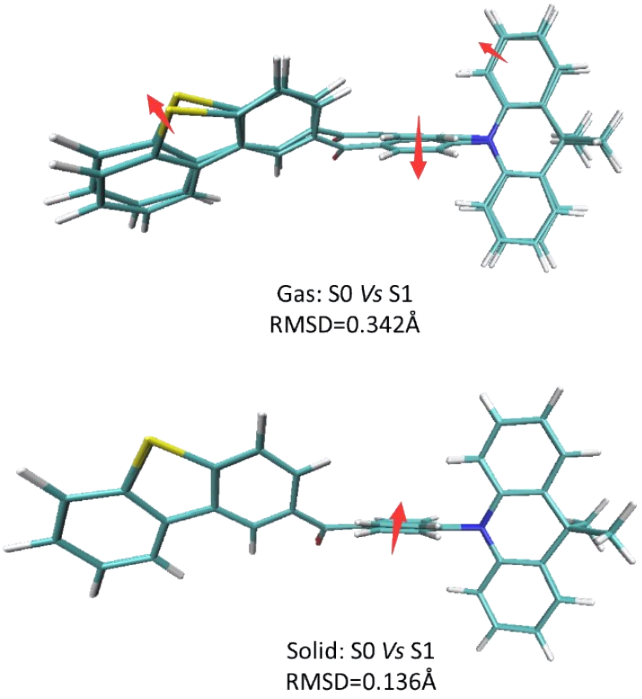


Figure S2. Geometry changes between S0 and S1 in gas and solid phase for configuration-1.



Configuration-2

Figure S3. Geometry changes between S0 and S1 in gas and solid phase for configuration-2.

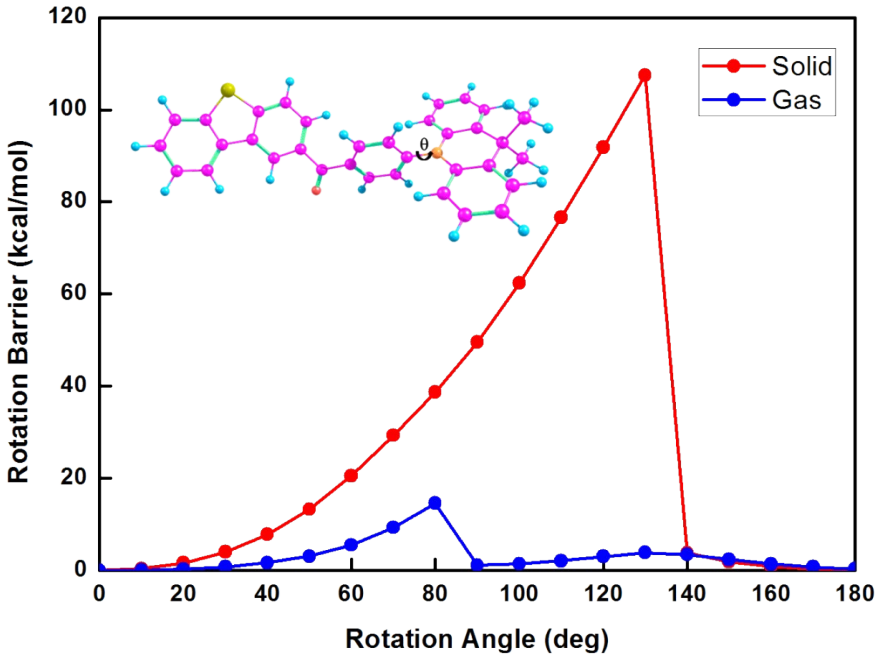


Figure S4. Rotational energy barriers (kcal/mol) obtained by rotating the dihedral angle θ marked in inset in gas (blue line) and solid phase (red line) respectively.

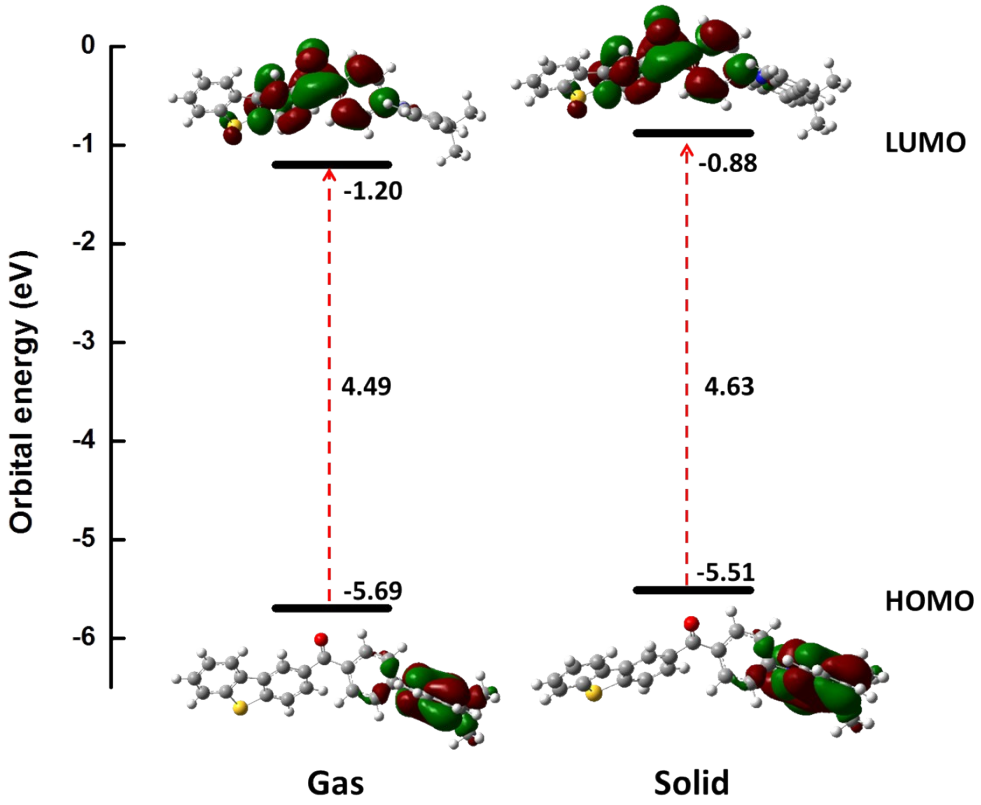


Figure S5. Frontier orbital distributions and their energy gaps of DBT-BZ-DMAC in gas and solid phase respectively.

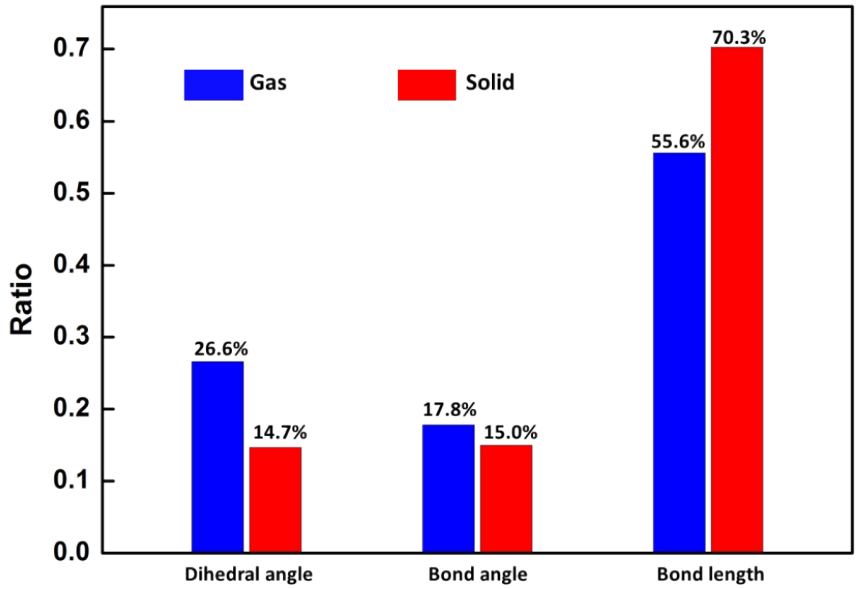


Figure S6. Contribution ratios to the reorganization energy from bond length, bond angle and dihedral angle of DBT-BZ-DMAC in gas and solid phase respectively.

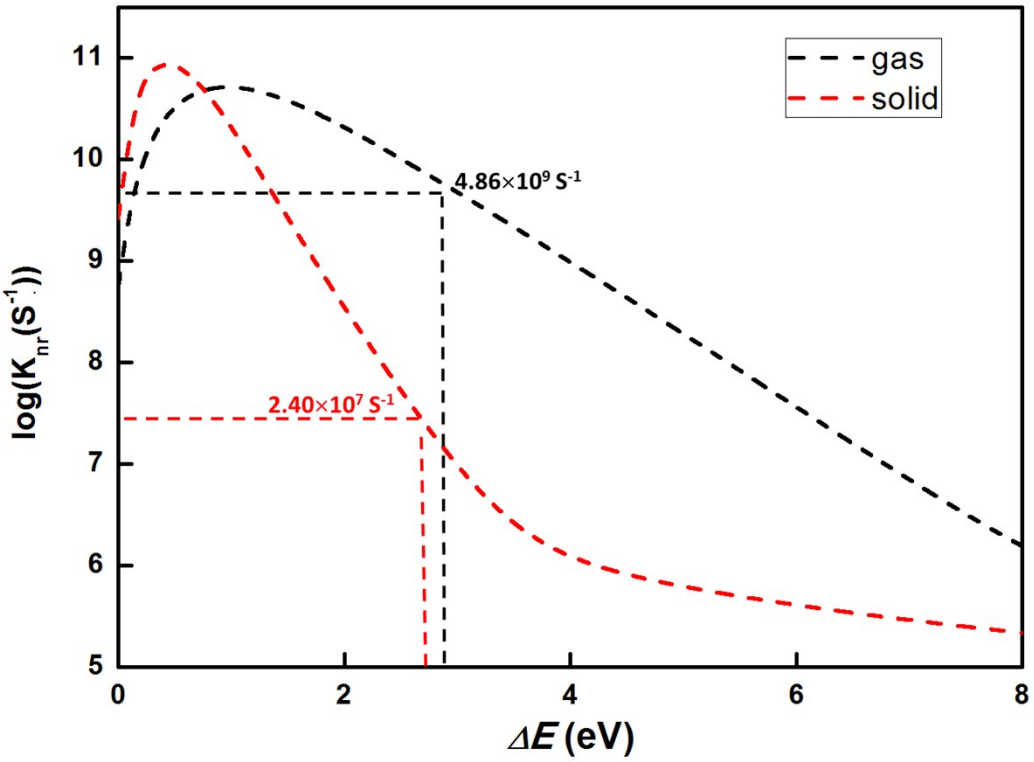


Figure S7. Non-radiative decay rate k_{nr} from S1 to S0 versus the adiabatic energy gap ΔE in gas (black) and solid phase (red) respectively.

Table S1. Geometry parameters of configuration-1 in gas and solid phase. θ, α and B represents the dihedral angle, bond angle and bond length respectively.

	Configuration-1						**Exp**
	Gas			**Solid**			
	S0	**S1**	**T1**	**S0**	**S1**	**T1**	**S0**
θ1	49.9	43.7	48.3	63.1	53.3	48.7	60.8
θ2	-86.3	-90.5	-96.3	-91.3	-99.5	-112.1	-93.9
θ3	152.3	145.2	148.4	148.2	142.8	143.8	145.5
θ4	149.5	165.8	157.5	138.2	154.7	159.6	143.8
α1	120.1	117.7	114.4	120.4	118.6	118.4	120.0
α2	119.6	121.4	117.5	119.6	121.2	120.7	119.7
α3	120.3	120.9	128.1	120.0	120.2	120.9	120.2
B 1	1.507	1.513	1.465	1.502	1.507	1.506	1.488
B 2	1.511	1.456	1.456	1.505	1.454	1.452	1.492
B 3	1.430	1.439	1.429	1.429	1.446	1.430	1.439

θ1: (2,4,6)&(26,27,29). θ2: 22-21-60-51. θ3: 4-6-20-61. θ4: 27-26-20-61.

α1: 6-20-61. α2: 26-20-61. α3: 6-20-26.

B1: 6-20. B2:20-26. B3:21-60.

Table S2. Geometry parameters of configuration-2 in gas and solid phase. θ, α and B represents the dihedral angle, bond angle and bond length respectively.

	Configuration-2						**Exp**
	Gas			**Solid**			
	S0	**S1**	**T1**	**S0**	**S1**	**T1**	**S0**
θ1	49.9	43.8	48.3	63.1	53.3	48.7	60.8
θ2	86.3	90.5	96.3	91.3	99.5	112.1	93.9
θ3	-152.4	-145.2	-148.4	-148.2	-142.8	-143.8	-145.5
θ4	-149.5	-165.8	-157.5	-138.2	-154.7	-159.6	-143.8
α1	120.1	117.7	114.4	120.4	118.6	118.4	120.0
α2	119.6	121.4	117.5	119.6	121.2	120.7	119.7
α3	120.3	120.9	128.1	120.0	120.2	120.9	120.2
B 1	1.507	1.513	1.465	1.502	1.507	1.506	1.488
B 2	1.511	1.456	1.456	1.505	1.454	1.452	1.492
B 3	1.430	1.439	1.429	1.429	1.446	1.430	1.439

θ1: (2,4,6)&(26,27,29). θ2: 22-21-60-51. θ3: 4-6-20-61. θ4: 27-26-20-61.
α1: 6-20-61. α2: 26-20-61. α3: 6-20-26.
B1: 6-20. B2:20-26. B3:21-60.