Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supplementary Information

Theoretical Investigation of Electronic Structure and Charge Transport Property of 9, 10-Distyrylanthracene (DSA) Derivatives with High Solid-State Luminescent Efficiency

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Hole **Electron**

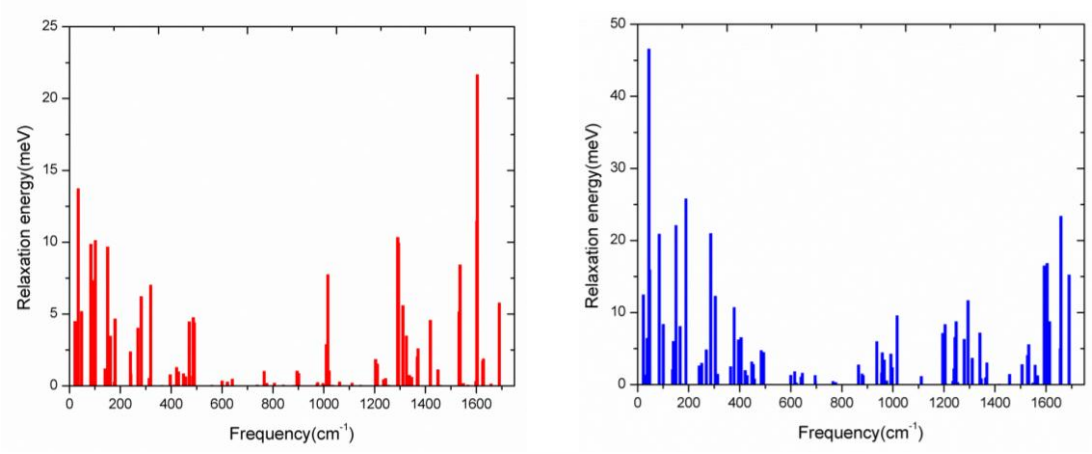

Figure S1. Contributions of the vibration modes to the relaxation energy in DSA-CN.

Hole **Electron**

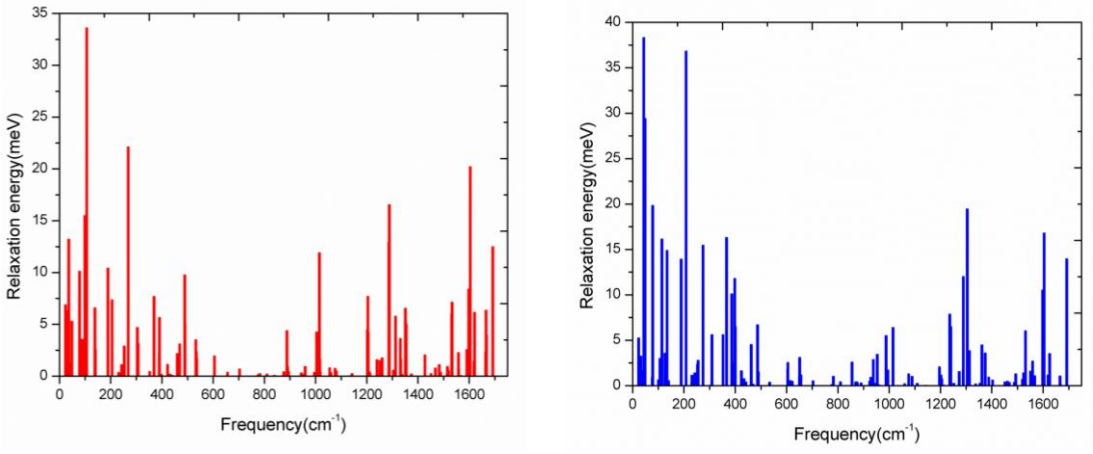

Figure S2. Contributions of the vibration modes to the relaxation energy in DSA-OCH_3.

Hole **Electron**

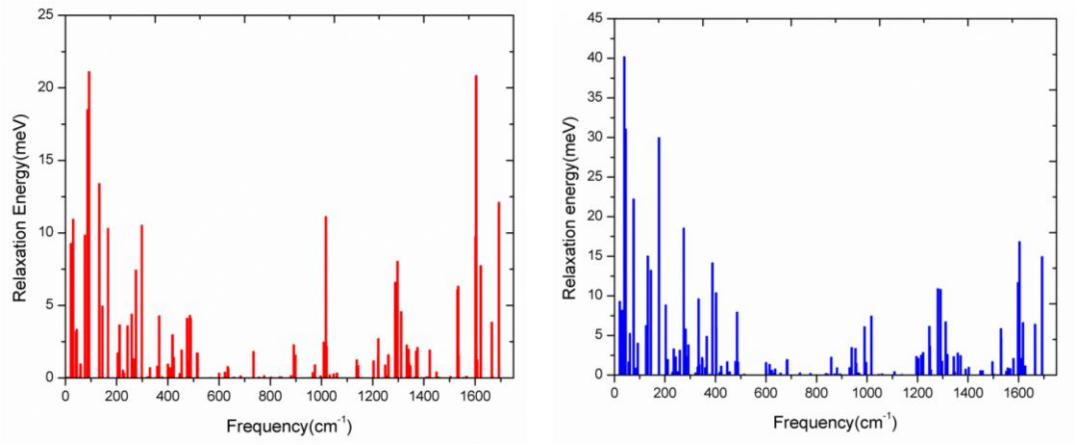

Figure S3. Contributions of the vibration modes to the relaxation energy in DSA-TBU.

(a) (b)

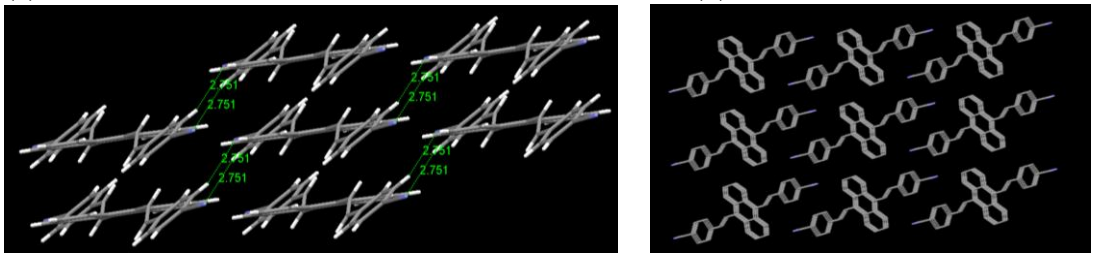

Figure S4. (a) The intermolecular interactions in the crystal of DSA-CN. The nearest intermolecular distance is 4.88 Å. (b) Crystal stacking motif of DSA-CN, viewed along the a-axis. The hydrogen atoms have been ellipsis for clarity.

(a) (b)

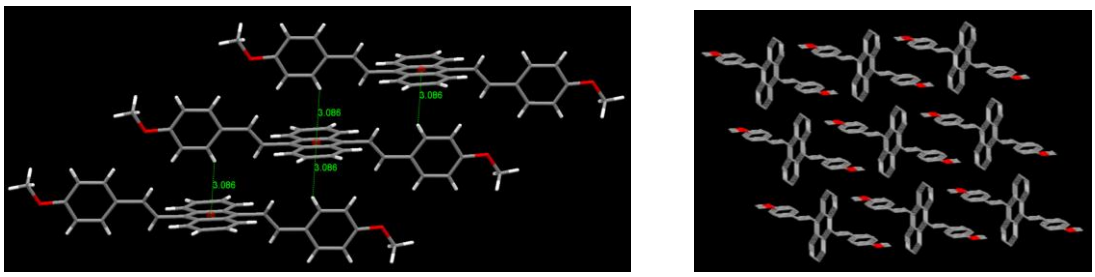

Figure S5. (a) The intermolecular interactions in the crystal of DSA-OCH_3. The nearest intermolecular distance is 6.96 Å. (b) Crystal stacking motif of DSA-OCH_3, viewed along the a-axis. The hydrogen atoms have been ellipsis for clarity.

(a) (b)

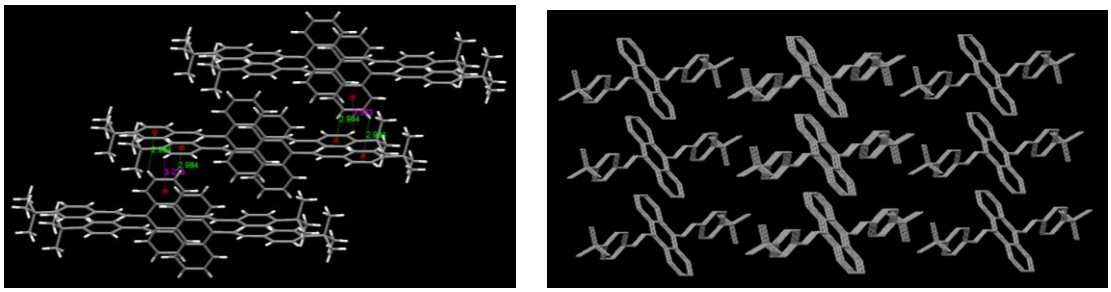

Figure S6. (a) The intermolecular interactions in the crystal of DSA-TBU. The nearest intermolecular distance is 6.2 Å. (b) Crystal stacking motif of DSA-TBU, viewed along the b-axis. The hydrogen atoms have been ellipsis for clarity.

Table S1 The Selective Transfer Integrals Calculated for Compounds in This Study with the PW91PW91/6-31G (d, p) Level.

Compd.	**Pathway**	**Distance(Å)**	**V_{hole}(meV)**	**$V_{electron}$(meV)**
DSA	7, 8	10.82	0.11	1.25
	9,10,11,12	11.67	0.54	0.74
	13,14,15,16	13.78	0.92	0.34
DSA-CN	3, 4	9.26	2.01×10^{-3}	2.17×10^{-3}
	9, 10	13.88	0.068	0.23
	13,14	16.54	7.6×10^{-4}	1.1×10^{-2}
DSA-OCH_3	3, 4	12.63	8.2×10^{-3}	0.59
	7, 8	9.74	0.15	0.09
	9, 10	16.82	0.048	0.011
	11, 12	12.00	0.04	0.05
	13, 14	10.47	9.2×10^{-5}	1.4×10^{-4}
DSA-TBU	5, 6	12.08	5.13×10^{-4}	6.97×10^{-4}
	9, 10	17.72	0.59	0.14
	11, 12	17.36	0.06	0.029
	13, 14	24.53	0.075	0.05
	15, 16	23.7	0.083	0.07