DFT Characteristics of Charge Transport in DBTP-Based Hole Transport Materials

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Table S1. Calculated transition energies, absorption peaks λ, major transition molecular orbitals and oscillator strength *f* of two molecules.

Molecules	State	Energy (eV)	λ (nm)	Transition MO	*F*
mDPA-DBTP	S1	3.51	352.87	H→L (0.66141)	1.9179
	S2	4.20	295.32	H-1→L (0.48622)	0.0098
	S3	4.24	292.22	H-2→L (0.37857)	0.0472
	S4	4.30	288.54	H→L+2 (0.46086)	0.0153
	S5	4.44	279.51	H-1→L+2 (0.33012)	0.5738
	S6	4.46	278.20	H→L+4 (0.44904)	0.0004
pTPA-DBTP	S1	3.47	357.45	H→L (0.59114)	3.3143
	S2	3.94	314.57	H-1→L (0.47473)	0.0142
	S3	4.23	293.41	H-1→L+2 (0.37815)	0.0286
	S4	4.23	292.86	H-1→L+3 (0.39074)	0.1055
	S5	4.25	291.56	H-3→L (0.52097)	0.0560
	S6	4.30	288.02	H-2→L (0.48100)	0.1547