Electronic Supplementary Material (ESI) for RSC Advances.

Bis(diphenylamino)naphthalene Host Materials: Careful Selection of the Substitution Pattern for the Design of Fully Solution-Processed Triple-Layered Electroluminescent Devices

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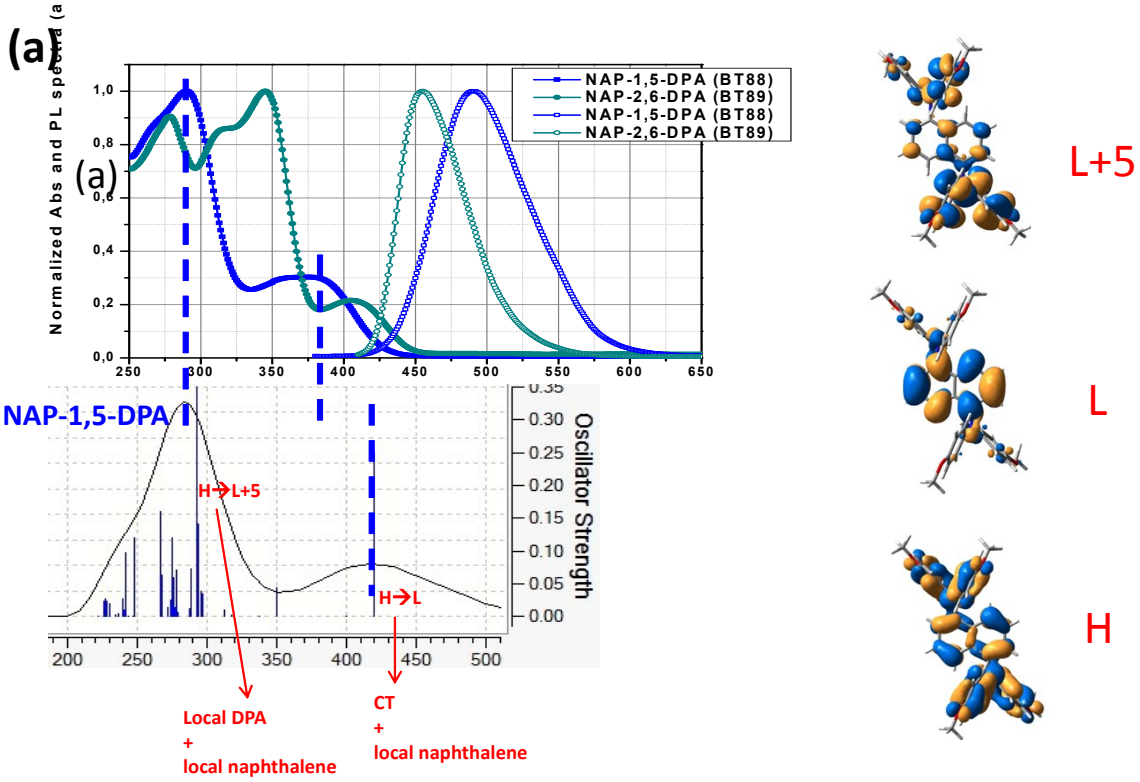
Supporting information



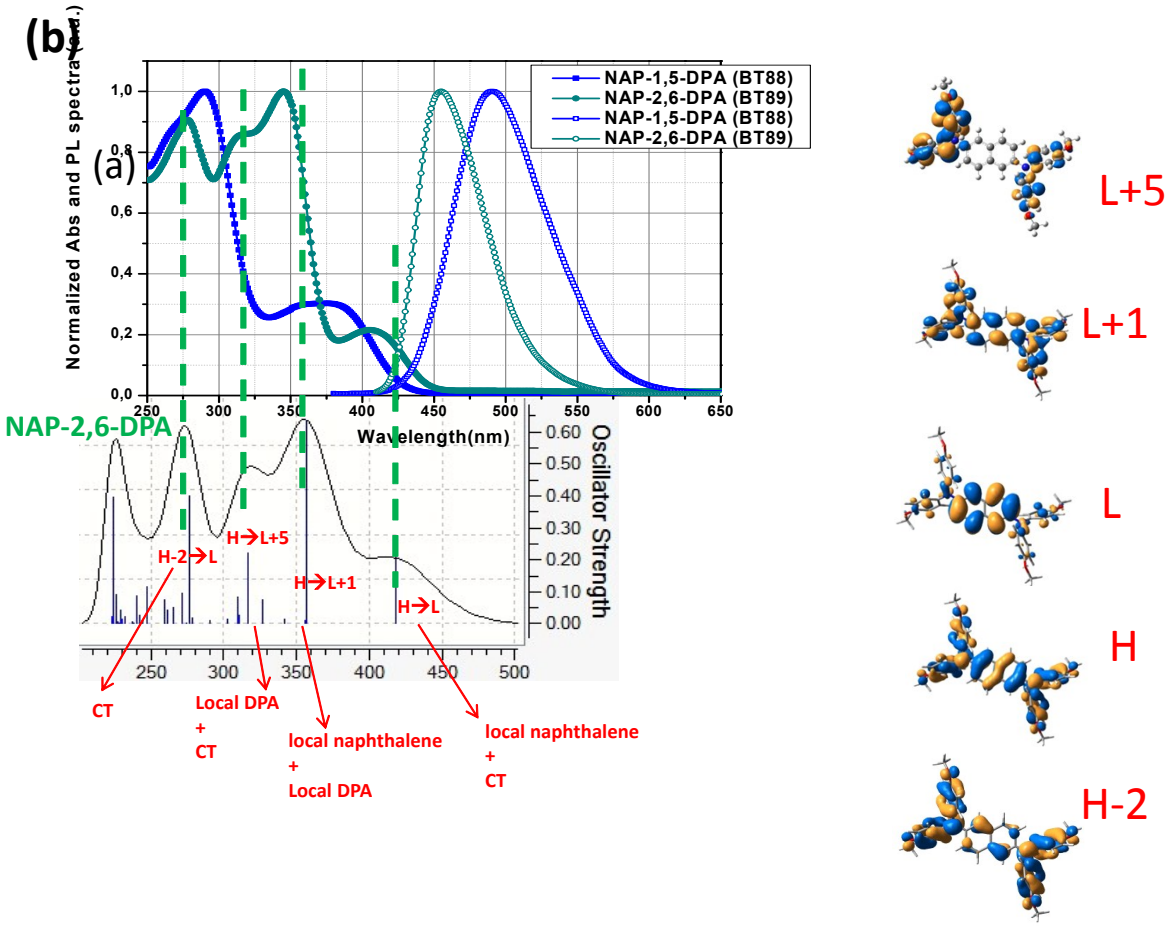


Figure S1. Experimental and theoretical absorption spectra of compounds **NAP-1,5-DPA** and **NAP-2,6-DPA**. The red shift of the theoretical low energy band for both compounds is due to the well-known bad performance of B3LYP (and other functionals containing low % of Hatree-Fock exchange) to correctly describe the CT transitions. Note the larger redshift (~40 nm) in the case of **NAP-1,5-DPA** (dominantly CT character), as compared to 13 nm in the case of **NAP-2,6-DPA** (dominantly local-naphthalene excitation character).

Table S1. Theoretical dipole moments (Debye) of compounds **NAP-1,5-DPA** and **NAP-2,6-DPA** and of the corresponding "half-compounds" (**NAP-1-DPA** and **NAP-2-DPA,** containing only one DPA substituent) in the ground state and the 1st excited state (vertical values). The dipole moments of the S1 state in the relaxed geometry are given in parentheses). All values are obtained at the B3LYP/6-31G(d,p) level in gas phase.

	GS	S_1
NAP-1,5-DPA	0.5	1.2 (15)
NAP-2.6-DPA	0.1	0.1 (0.2)
NAP-1-DPA	2.1	12.8
NAP-2-DPA	3.0	11.9