Electronic Supplementary Material (ESI) for RSC Advances.

Phenothiazine Derivates Based D-π-A and D-A-π-A Organic Dye for Dye-Sensitized Solar Cells

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Table SI TD-DFT (CAMB3LYP) calculated data of **JH305** and **JH307**

Dyes	State	Composition [a]	*E*(eV)	*f* [b]	exp.(eV, nm)
JH305	S_1	H→L (53%) H–1→L (34%) H–2→L (15%) H→L+1 (16%)	2.71 eV (457 nm)	1.6319	2.71 eV (457nm)
	S_2	H→L (33%) H–1→L (41%) H–2→L (29%) H–4→L (10%) H–5→L (12%)	3.5 eV (354 nm)	0.0538	3.43 eV (361 nm)
JH307	S_1	H→L (59%) H–1→L (31%) H–2→L (14%) H→L+1 (14%)	2.4 eV (517 nm)	1.0052	2.49 eV (498 nm)
	S_2	H→L (29%) H–1→L (41%) H–2→L (42%) H→L+1 (16%)	3.12 eV (396 nm)	0.3042	3.02 eV (410 nm)

(a) H=HOMO, L= LUMO, H–1=HOMO–1, H–2=HOMO–2, H–4=HOMO–4, H–5=HOMO–5, L+1= LUMO+1.(b) oscillator strengths