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Characterizations of Efficient Charge Transfer and Photoelectric Performance in the Cosensitization of Solar Cells

Qian Liu [1,2], Xiaochen Lin [3], Lu Mi [2], Nan Gao [2], Peng Song [4,*], Fengcai Ma [4,] and Yuanzuo Li [2,*]

[1] Department of Applied Physics, Xi'an University of Technology, Xi'an 710054, China; liuqian@xaut.edu.cn
[2] College of Science, Northeast Forestry University, Harbin 150040, China; milufine@sina.com (L.M.); nan_g@nefu.edu.cn (N.G.)
[3] Chemical Industry and Material College, Heilongjiang University, Harbin 150080, China; xiaochenlinhd@sohu.com
[4] Department of Physics, Liaoning University, Shenyang 110036, China; mafengcai@lnu.edu.cn
* Correspondence: yzli@nefu.edu.cn (Y.L.); songpeng@lnu.edu.cn (P.S.); Tel: +86-451-8219-2245 (Y.L.); Tel.: +86-24-62202365 (P.S.).

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Supplementary materials

Table S1 The HOMO (highest occupied molecular orbital), LUMO (lowest unoccupied molecular orbital) and energy gap for D35, XY1 and D35&XY1.

levels	D35	D35/TiO_2	XY1	XY1/TiO_2	D35+XY1
H	-5.03	-4.97	-4.81	-4.81	-4.81
L	-2.75	-2.81	-2.83	-2.89	-2.82
Gap	-2.28	-2.16	-1.98	-1.92	1.99

Table S2. The main excited states for dyes in acetonitrile solvent, adsorption of TiO2 and co-sensitization.

Dyes	wavelength(nm)	E(eV)	Strength f	CI coefficient
D35	453	2.74	1.36	H→L（76%）
	299	4.15	1.02	H→L+2（74%）
D35-TiO2	458	2.71	1.58	H→L（57%）
	298	4.16	0.92	H→L+23（38%）
XY1	529	2.34	2.19	H→L（62%）
XYI-TiO2	538	2.30	2.33	H→L（54%）
	302	4.11	1.03	H→L+24（38%）
D35&XY1	530	2.34	1.95	H→L（58%）
	455	2.72	1.20	H-1→L+1(67%)

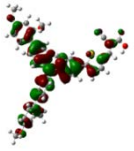
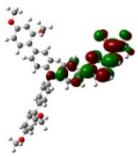
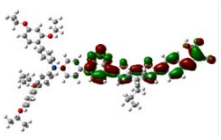
Table S3. Absorption spectra data for the dyes in the different field.

Field	states.	eV (nm)	f	Configuration	CI coefficient
0	S_1	2.3413 (529.55)	1.9536	H→L	0.54048
	S_2	2.7233 (2.7233)	1.2035	H-1→L+1	0.57916
	S_3	2.9085 (426.28)	0.4613	H→L+2	0.49349
	S_4	3.2669 (379.52)	0.1408	H-2→L+2	0.44156

10	S_5	3.2920 (376.62)	0.0001	H-1→L	0.66670
	S_6	3.4350 (360.94)	0.0006	H→L+1	0.59498
	S1	2.3132 (535.99)	1.7157	H-1→L	0.66292
	S2	2.8868 (429.49)	1.0777	H→L+1	0.59865
	S3	3.0405 (407.77)	0.8422	H-1→L+2	0.56707
	S4	3.0840 (402.02)	0.0039	H→L	0.68930
	S5	3.4390 (360.53)	0.3300	H-2→L	0.59101
	S6	3.6255 (341.98)	0.0011	H→L+2	0.65257
20	S1	2.1996 (563.65)	1.5047	H-1→L	0.65265
	S2	2.7203 (455.78)	0.0003	H→L	0.68909
	S3	3.0121 (411.62)	0.8734	H→L+3	0.56259
	S4	3.1152 (397.99)	1.2719	H-1→L+2	0.58938
	S5	3.4928 (354.97)	0.4112	H-4→L	0.54678
	S6	3.5701 (347.29)	0.0021	H→L+2	0.51533
30	S1	2.0287 (611.14)	1.3827	H-1→L	0.64359
	S2	2.2824 (543.21)	0.0006	H→L	0.68599
	S3	3.0895 (401.30)	0.1804	H→L+9	0.48358
	S4	3.1422 (394.57)	2.0640	H→L+9	0.44971
	S5	3.1867 (389.07)	0.0003	H→L+1	0.68172
	S6	3.2250 (384.45)	0.0017	H-2→L	0.61677

Table S4 Estimated Electrochemical Parameters for the dyes.

Dye	ΔG^{inject} **(eV)**	**LHE**	E_{dye*} **(eV)**	E_{dye} **(eV)**	μ_{normal} **(D)**	**E_{ads}**	**t/ns**
D35	-1.70687	0.9563	2.293129	-5.03113	13.9281	-4.03	2.27
XY1	-1.53669	0.9935	2.463307	-4.80801	-17.1053	-4.04	1.92
XY&D35	-1.6103	0.9889	2.389703	-4.731	27.3679		

.orbitals.	D35	XY1
HOMO-1		
HOMO		
LUMO		

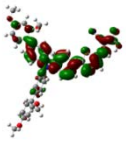
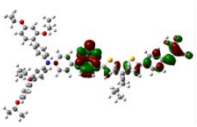
LUMO+1		

Figure S1 The frontier molecular orbital for D35 and XY1, respectively.