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苯并噻二唑衍生物作为铆接基团提高染料敏化太阳能电池效率

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Design of Benzobisthiadiazole Analogues as Promising Anchoring Groups for High Efficient Dye-Sensitized Solar Cells

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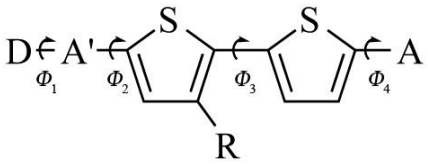
Table S1 Calculated dihedral angles between the neighbouring units of dyes.



	SPC	SPN	SPO	SPS	SPSe
Φ_1	34.41	35.02	34.52	34.81	34.85
Φ_2	5.07	5.37	5.35	5.25	5.02
Φ_3	-2.95	-7.16	-2.84	-4.24	-3.35
Φ_4	-0.08	0.03	0.03	0.02	0.09

Φ_1-Φ_4 represent the dihedral angles, the unit is °.

Table S2 Main electron transitions, oscillator strengths (*f*) and absorption bands with *f* > 0.1 and λ > 350nm in the visible and near-UV regions for all the dyes in CH_2Cl_2.

Sensitizer	Excited energy/eV	λ/nm	*f*	composition		LHE
SPC	1.186(S_0-S_1)	1045.2	0.67	H → L (75.65%)	H − 1 → L (22.58%)	0.79
	2.186(S_0-S_2)	567.1	0.67	H − 1→ L (40.65%)	H − 2 → L (24.68%)	
	2.569(S_0-S_3)	482.7	0.42	H → L + 1 (71.24%)	H − 2 → L + 1 (6.80%)	
	2.752(S_0-S_4)	450.5	0.11	H − 2 → L (46.39%)	H − 1 → L (27.84%)	
SPN	1.973 (S_0-S_1)	628.4	1.22	H → L (59.48%)	H − 1 → L (31.89%)	0.94
	2.524 (S_0-S_2)	491.2	0.53	H → L + 1 (74.09%)	H − 1 → L (10.81%)	
	3.220(S_0-S_4)	385.1	0.12	H − 1 → L + 1 (53.26%)	H − 2 → L (18.87%)	
SPO	1.540 (S_0-S_1)	805.3	0.99	H → L (56.39%)	H − 1 → L (38.74%)	0.90
	2.381(S_0-S_2)	520.7	0.55	H → L + 1 (33.57%)	H − 1 → L (26.78%)	
	2.652 (S_0-S_3)	467.4	0.25	H → L + 1 (53.97%)	H → L (19.38%)	
SPS	1.622 (S_0-S_1)	764.4	0.89	H → L (59.84%)	H − 1 → L (34.46%)	0.87
	2.447(S_0-S_2)	506.7	0.74	H → L + 1 (59.35%)	H − 1 → L (15.60%)	
SPSe	1.472 (S_0-S_1)	842.2	0.75	H → L (65.79%)	H − 1 → L (29.54%)	0.82
	2.393(S_0-S_2)	518.1	0.78	H → L + 1 (44.30%)	H − 1 → L (21.73%)	
	2.646(S_0-S_3)	468.6	0.16	H → L + 1 (42.51%)	H − 1 → L (18.76%)	
	3.473(S_0-S_6)	357.0	0.40	H − 7 → L (41.85%)	H − 8 → L (41.57%)	
WS-9	2.34(S_0-S_1)	529 (536)[a]	1.81	H → L (65.6%)	H − 1 → L (19.37 %)	0.98
	2.92(S_0-S_2)	424	0.20	H → L + 1(43.8%)	H − 1 → L (38.1%)	

[a]Data are experimental values from Ref.39.

Table S3 Calculated adsorption energies (in eV) and corresponding bond lengths (in nm)

	SPC	SPN	SPO	SPS	SPSe	WS-9
E_{ads}	−5.43	−4.11	−4.70	−4.70	−4.92	−6.13
d(Ti-N/O)$_1$	0.204	0.206	0.207	0.206	0.202	0.190
d(Ti-N/O)$_2$	0.208	0.211	0.208	0.207	0.206	0.194