

Novel coumarin sensitizers based on 2-(thiophen-2-yl)thiazole π - bridge for dye-sensitized solar cell

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Table SI Electrochemical properties of coumarin dyes

Compd	Experimental ^a (eV)			Calculated ^d (eV)		
	HOMO ^a	E ₀₋₀ ^b	LUMO ^c	HOMO	E ₀₋₀	LUMO
ZXY-a	-4.82	2.35	-2.47	-5.40	2.47	-2.93
ZXY-b	-4.74	2.27	-2.47	-5.27	2.41	-2.86

^a The oxidation potential E_{ox} in DMF was determined from cyclic voltammograms and used to describe the ground-state energy HOMO; ^b E₀₋₀ was calculated from E₀₋₀ = 1240/ λ_{int} and λ_{int} was the intersection of the normalized absorption and emission spectra; ^c E_{LUMO} was calculated from E_{ox}-E₀₋₀; ^d Calculated at the B3LYP/6-31G(d) level.