Supporting Information

An attempt to improve the performance of pyrrole-containing dyes in dye sensitized solar cells by adjusting isolation groups

Huiyang Li,[a] *Yingqin Hou,*[a] *Yizhou Yang,*[a] *Runli Tang,*[a] *Junnian Chen,*[a] *Heng Wang,*[b] *Hongwei Han,*[b] *Tianyou Peng,*[a] *Qianqian Li**[a] *and Zhen Li**[a]

[a] Department of Chemistry, Hubei Key Lab on Organic and Polymeric Opto-Electronic Materials, Wuhan University, Wuhan 430072, China

[b]Michael Grätzel Center for Mesoscopic Solar Cells, Wuhan National Laboratory for Optoelectronics, Huazhong University of Science and Technology, Wuhan, 430072, China

Corresponding author. Phone: 86-27-62254108; Fax: 86-27-68756757; E-mail: qianqian-alinda@163.com, lizhen@whu.edu.cn, or lichemlab@163.com.

Table S1 Dye sensitized solar cell performance data of dyes

sensitizer	CDCA (mM)	J_{sc} (mA cm^{-2})	V_{oc} (V)	*FF*	η (%)
LI-54	0	11.30	0.69	0.66	5.12
	5	12.23	0.72	0.61	5.36
	10	12.45	0.73	0.62	5.59
LI-55	0	12.61	0.72	0.65	5.94
	5	13.51	0.74	0.63	6.30
	10	13.49	0.72	0.61	5.92
LI-56	0	12.60	0.70	0.67	5.88
	5	13.69	0.72	0.60	5.94
	10	12.72	0.74	0.62	5.88
LI-57	0	13.85	0.72	0.64	6.43
	5	13.49	0.72	0.63	6.11
	10	12.92	0.75	0.59	5.76

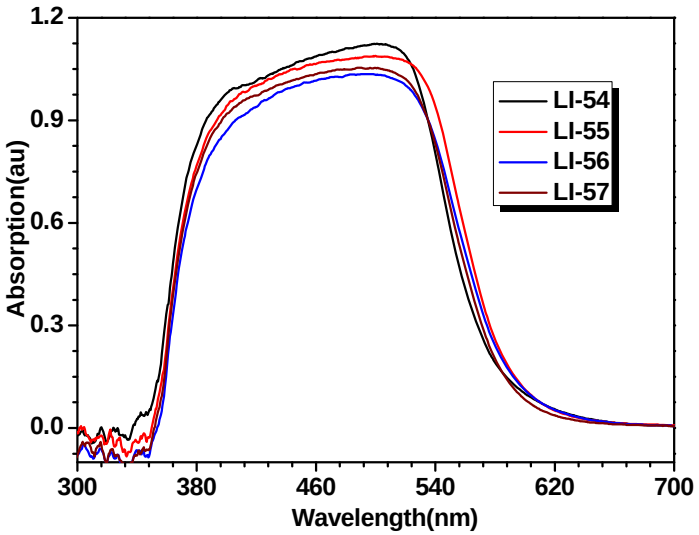

Figure S1. UV-vis spectra of the sensitizers on TiO_2 films.

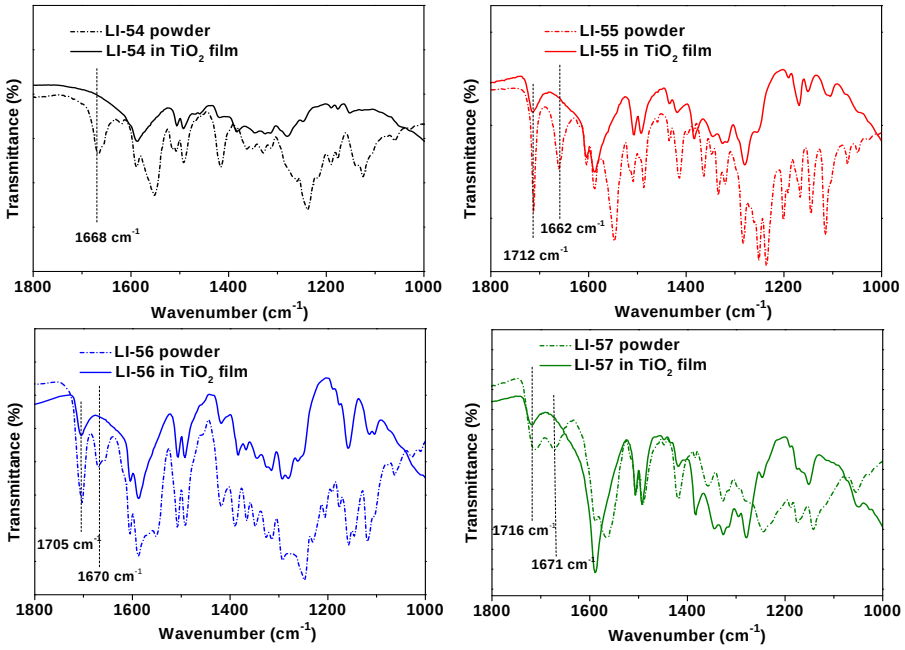

Fig. S2 IR spectra of the four pyrrole-containing dyes

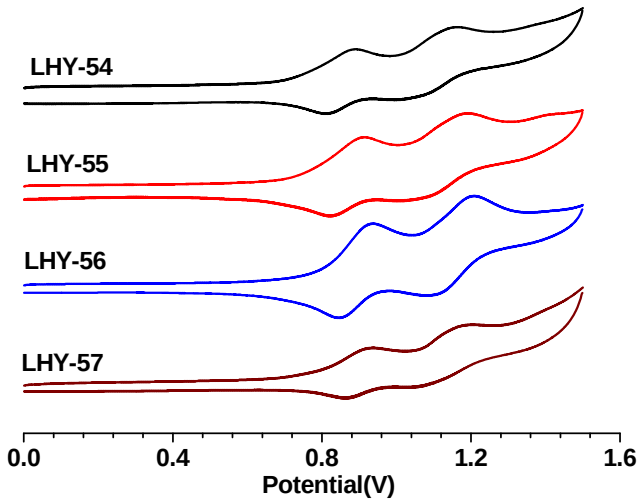

Figure S3. Cyclic voltammograms of sensitizers in CH_2Cl_2.

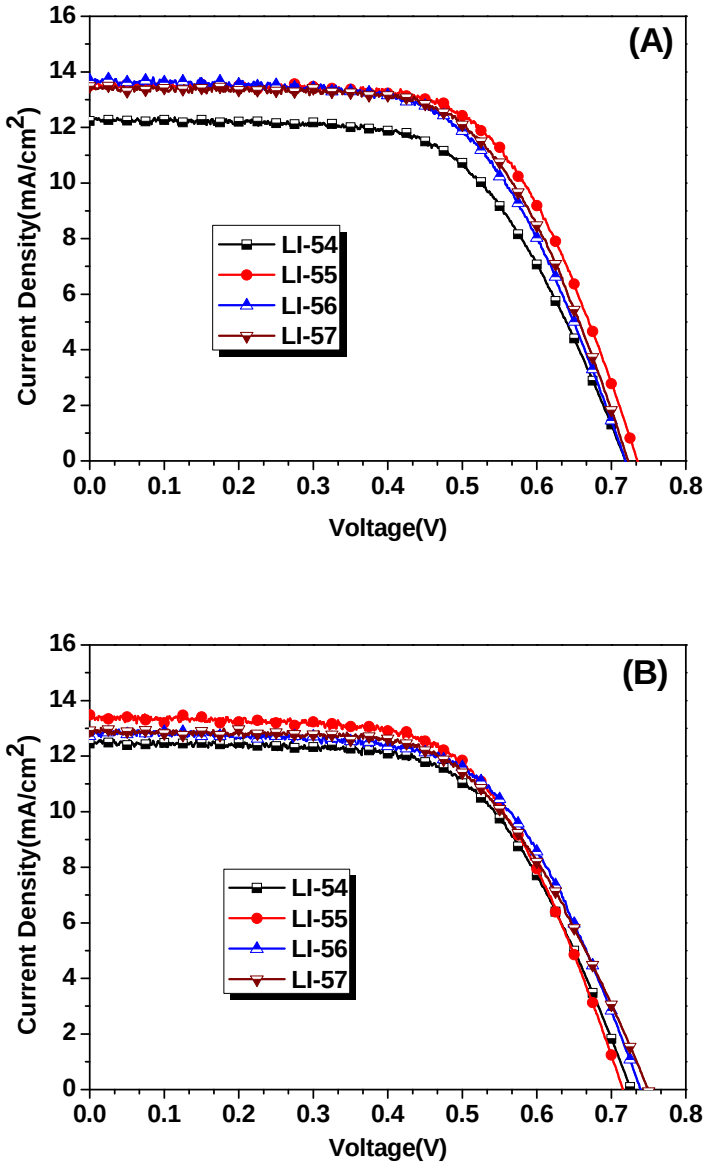

Figure S4. *J*-V characteristics of DSCs measured at simulated 100 mWcm^{-2}AM1.5 conditions. (A) The TiO_2 electrode (0.238 cm^2) was stained by immersing it into the CDCA solution (5 mM) for 6 h, then to the dye solution (0.3 mM) in CH_2Cl_2 for 24 h, (B) The TiO_2 electrode (0.238 cm^2) was stained by immersing it into the CDCA solution (10 mM) for 6 h,then to the dye solution (0.3 mM) in CH_2Cl_2 for 24 h.

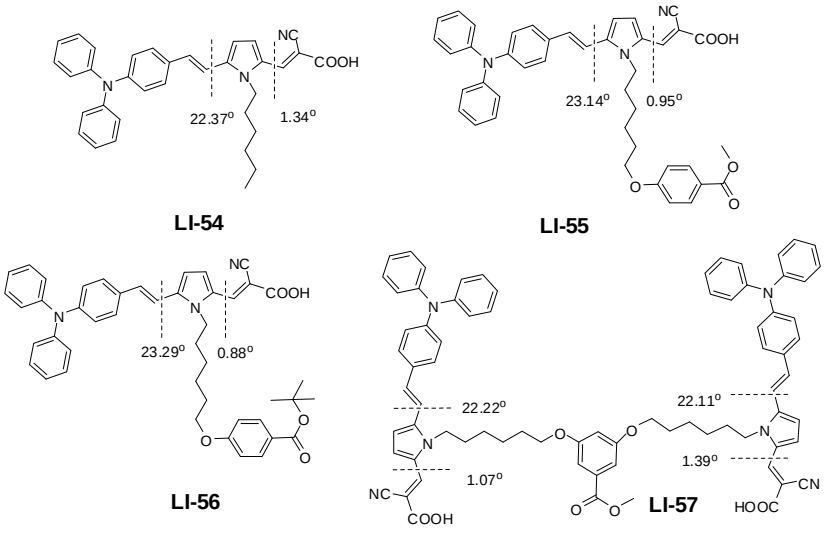

Figure S5. Dihedral angles between pyrrole unit and its neighboring units