

# Coplanar Donor- $\pi$ -Acceptor Dyes Featuring a Furylethynyl Spacer for Dye-Sensitized Solar Cells

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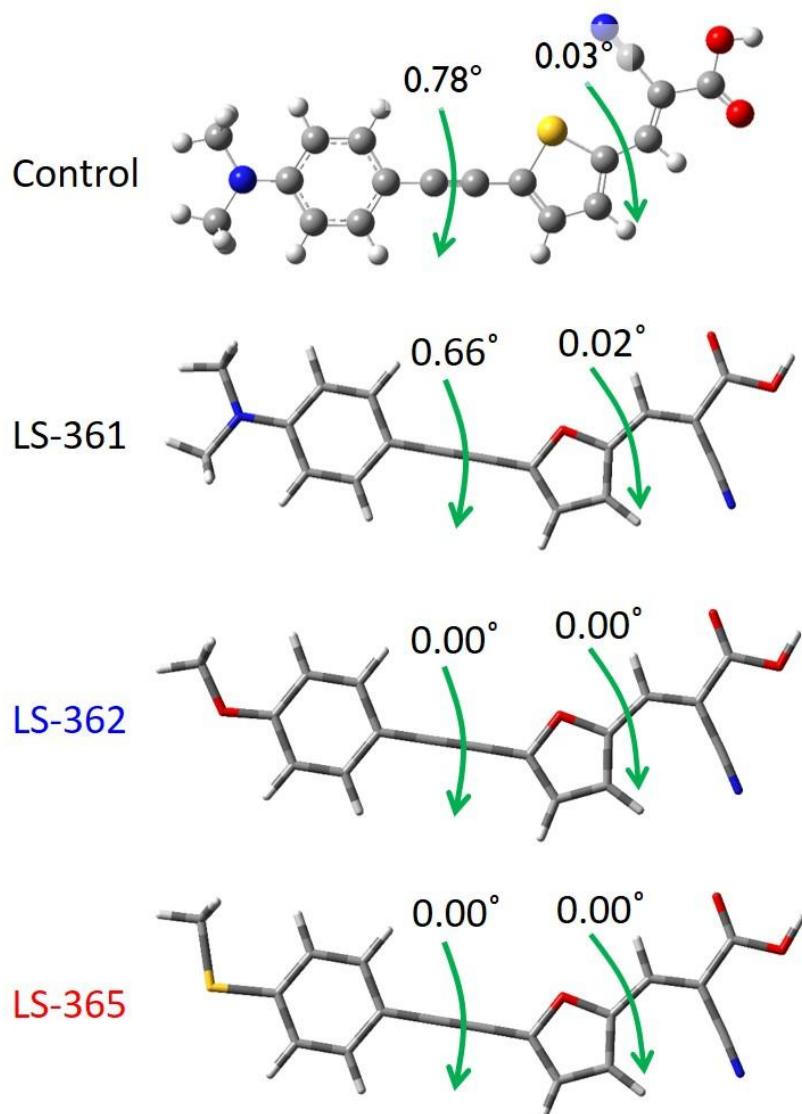
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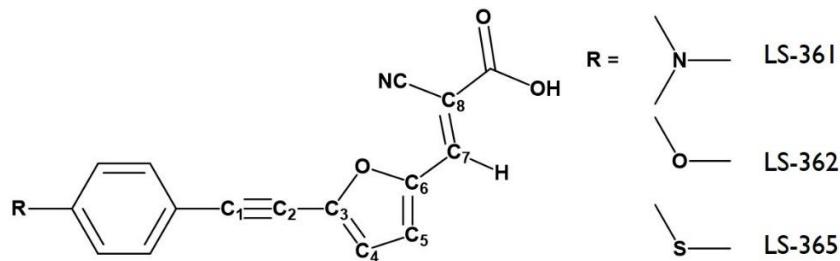
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Received: 14 February 2019; Accepted: 4 March 2019; Published: 12 March 2019



**Figure S1.** Optimized molecular geometries of the three dyes (LS-361, LS-362 and LS-365).

**Table S1.** Conjugative interaction energies ( $\Delta E$ ) between the  $\pi$  and  $\pi^*$  orbitals in LS-361, LS-362 and LS-365 from the second-order perturbation theory analysis of the Fock matrix within the NBO analysis.



Dye	Donor Orbital	Acceptor Orbital	$\Delta E$ (kcal/mol)	$E_{\text{acc}} - E_{\text{don}}$ (a.u.)	$F(\text{acc}, \text{don})$ (a.u.)
<b>LS-361</b>	$\pi(C1 \equiv C2)$	$\pi^*(C3 = C4)$	16.86	0.30	0.066
	$\pi(C5 = C6)$	$\pi^*(C7 = C8)$	23.31	0.29	0.075
<b>LS-365</b>	$\pi(C1 \equiv C2)$	$\pi^*(C3 = C4)$	15.94	0.30	0.065
	$\pi(C5 = C6)$	$\pi^*(C7 = C8)$	22.38	0.30	0.073
<b>LS-362</b>	$\pi(C1 \equiv C2)$	$\pi^*(C3 = C4)$	16.18	0.30	0.065
	$\pi(C5 = C6)$	$\pi^*(C7 = C8)$	22.63	0.30	0.074
<b>Control</b>	$\pi(C1 \equiv C2)$	$\pi^*(C3 = C4)$	15.82	0.29	0.064
	$\pi(C5 = C6)$	$\pi^*(C7 = C8)$	25.26	0.30	0.080

**Table S2.** The NBO population charge for electron donor,  $\pi$ -bridge and electron acceptor, which denoted as  $q^{\text{donor}}$ ,  $q^{\pi\text{-bridge}}$  and  $q^{\text{acceptor}}$ , respectively.  $\Delta q^{D-A}$  represents the charge variance between natural charges on the donor and acceptor groups.

Dye	$q^{\text{donor}}$	$q^{\pi\text{-bridge}}$	$q^{\text{acceptor}}$	$\Delta q^{D-A}$
<b>LS-361</b>	0.0797	0.1037	-0.1835	0.2632
<b>LS-362</b>	0.0492	0.1173	-0.1665	0.2157
<b>LS-365</b>	0.0387	0.1223	-0.1610	0.1997
<b>Control</b>	0.0836	0.0894	-0.1729	0.2565

**Table S3.** EIS fitting parameters estimated from the EIS spectra in Figure 4(c).

Dye	$R_{tr}$ ( $\Omega$ )	$R_{rec}$ ( $\Omega$ )	$C_{\mu}$ (mF)	$\tau_e$ (ms)	$\eta_{cc}$ (%)
<b>LS-361</b>	11.26	75.91	0.05	3.56	87.08
<b>LS-362</b>	10.09	126.00	0.03	3.56	92.59
<b>LS-365</b>	14.75	85.08	0.03	2.52	85.22
<b>Control</b>	7.45	92.51	0.04	3.56	93.64