

**Supporting Information for**  
**Control and regulation of the performance of fullerene-**  
**based dye-sensitized solar cells with D-D-A structure by**  
**external electric fields**

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**Table S1.** Dipole moment of the molecule in  $F_{\text{ext}}$  ( $F_{\text{ext}}$  in  $10^{-5}$  a.u.).

	$F_{\text{ext}}=-10$	$F_{\text{ext}}=0$	$F_{\text{ext}}=10$
Dipole moment of the molecule (Debye)	9.9197	10.6164	11.3247

**Table S2.** Electronic transition energy ( $\Delta E$ ), absorption wavelength( $\lambda_{\text{max}}$ ) and oscillator strength ( $f$ ) of Dye molecule.

<i>State</i>	$\Delta E/\text{eV}$	$\lambda_{\text{max}}/\text{nm}$	$f$
1	2.3308	531.94	0.0057
2	2.4245	511.38	0.0001
3	2.4573	504.55	0.0000
4	2.4825	499.44	0.0000
5	2.6868	461.45	0.0007
6	2.7326	453.72	0.0205
7	2.7382	452.79	0.1752
8	2.7440	451.83	0.3707
9	2.7838	445.38	0.0005
10	2.8781	430.79	0.0035
11	2.9357	422.34	0.0060
12	2.9515	420.07	1.5667
13	2.9724	417.12	0.0014
14	2.9979	413.57	0.0004
15	3.0277	409.50	0.5095