January 27, 2015

Supporting Information: (one page)

Manuscript ID: RA-ART-11-2014-014620

Title: Dye Sensitized Solar Cell With Lawsone Dye Using Zno Photoanode: Experimental and TD-DFT Study.

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Supporting Information

Table S1: Theoretical UV-Vis absorption wavelengths of hydrogen-bonded lawsone with explicit ethanol molecule in ethanol calculated at TD/C-PCM/PBE1PBE/6-311+G(d,p) level of DFT. (H:HOMO, L:LUMO). The f values are oscillator strengths.

Lawsone with Explicit ethanol		
	λ (nm)	f
1.	289.6	0.3014
2.	332.7	0.0914
3.	400.4	0.0097
4.	409.6	0.0000

Table S2: Theoretical UV-Vis absorption wavelengths of a hydrogen-bonded lawsone dimer in ethanol calculated at TD/C-PCM/PBE1PBE/6-311+G(d,p) level of DFT. (H:HOMO, L:LUMO). The f values are oscillator strengths.

Lawsone dimer		
	λ (nm)	f
1.	291.7	0.3701
2.	305.3	0.0011
3.	322.8	0.0031
4.	331.6	0.0957
5.	337.0	0.0743
6.	352.7	0.0057
7.	392.3	0.0109
8.	394.9	0.0227
9.	397.3	0.0000
10.	407.6	0.0000