Electronic Supporting Information

Metal-Free Organic Dyes Containing Thiadiazole Unit for Dye-Sensitized Solar Cells: A Combined Experimental and Theoretical Study

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Table **S1** Absorption maxima (λmax), oscillator strength (f),main orbital transitions, coefficients of wave functions(CI) calculated at CAM-B3LYP and M062X/6-311+g(d,p) level in chloroform phase and ground state dipole moment calculated at B3LYP/6-311g(d,p) level for dyes **9** to **12**.

Dye	**λ_{max} (nm)**	**f**	**μ_{gs} (Dy)**	**CI**
9	453 (452)	2.174 (2.122)	12.26	0.520 (0.436) (H-1→L),-0.395 (0.486) (H→L)
10	465 (464)	2.416 (2.392)	8.66	0.55 (0.535) (H-1→L),0.35 (0.392) (H→L)
11	432 (430)	2.196 (2.207)	7.42	0.467 (0.44) (H-1→L) 0.45 (0.48) (H→L),
12	425 (423)	2.242 (2.234)	8.88	0.468 (0.484) (H-1→L), 0.45 (0.436) (H→L)

M06-2X values are given in parentheses

Table **S2** Absorption maxima (λmax), oscillator strength (f),main orbital transitions, coefficients of wave functions(CI) calculated using LC-BLYP, LC-WPBE, and WB97XD functional and 6-311+g(d,p) basis set in chloroform for dyes **9** to **12**.

Dye	LC-BLYP		LC-WPBE		WB97XD	
	λ_{max} in nm(f)	CI	λ_{max} in nm(f)	CI	λ_{max} in nm(f)	CI
9	404	0.58 (H-1→L)	405	0.576 (H-1→L)	438	0.556 (H-1→L)
	(2.092)	-0.27 (H→L)	(2.151)	-0.273 (H→L)	(2.232)	-0.327 (H→L)
10	410	0.571 (H-1→L)	414	0.576 (H-1→L)	451	0.569 (H-1→L)
	(2.351)	0.267 (H→L)	(2.387)	0.264 (H→L)	(2.433)	0.307 (H→L)
11	384	0.507 (H-1→L)	386	0.505 (H-1→L)	420	0.489 (H-1→L)
	(2.116)	0.364 (H→L)	(2.188)	0.3681 (H→L)	(2.227)	0.414 (H→L)
12	377	0.522 (H-1→L)	379	0.519 (H-1→L)	412	0.498 (H-1→L)
	(2.179)	-0.350 (H→L)	(2.255)	-0.356 (H→L)	(2.295)	0.403 (H→L)

Table **S3** Absorption and emission, properties of the synthesized dyes **9-12**

Dye	[a]λ_{max}/nm ($M^{-1}cm^{-1}$)	[b]λ_{max}/nm
9	440 (14995)	598
10	468 (8275)	576
11	435 (12386)	566
12	433 (15759)	542

[a]Absorption maximum. [b]Fluorescence emission maxima in $1x10^{-5}$ M acetonitrile:tert-butyl alcohol (1:1) solvent mixture

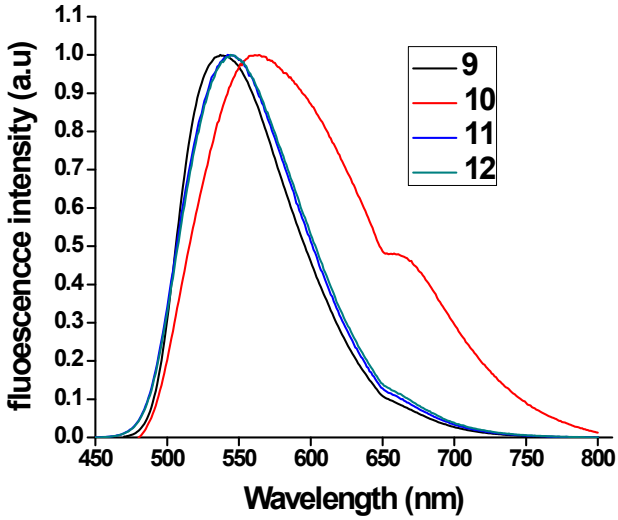

Fig. S1 Normalized emission spectra of **9-12** in $CHCl_3$

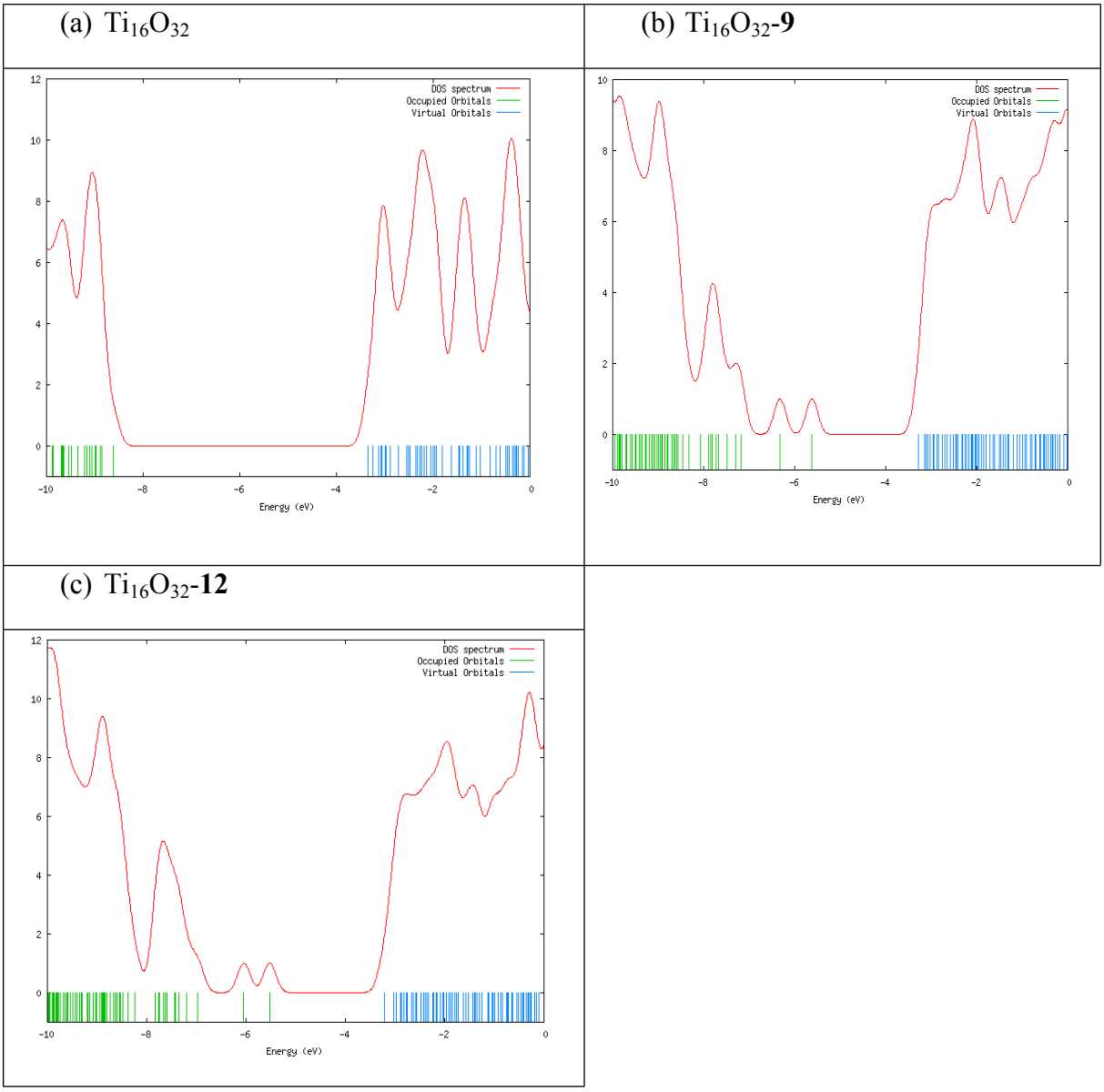

Fig. S2 DOS pictures obtained from GaussSum software on PBE0/TZVP optimized geometries (a) $Ti_{16}O_{32}$ (b) $Ti_{16}O_{32}$-**9** and (c) $Ti_{16}O_{32}$-**12**

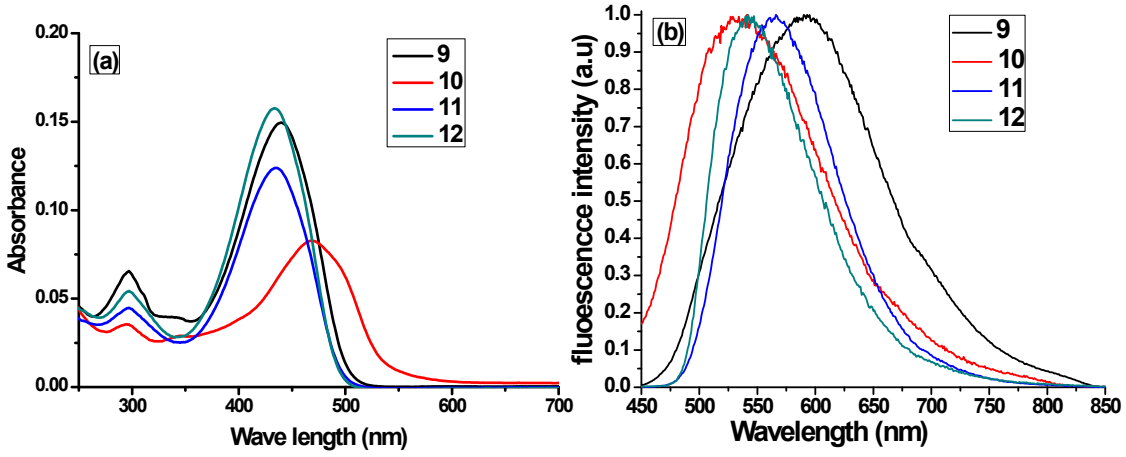

Fig. S3 The (**a**) UV-visible spectra and (**b**) Normalized emission spectra of **9-12** in $1x10^{-5}$ M in acetonitrile:tert-butyl alcohol (1:1) solvent mixture