Supporting Information for

Anti-aggregation and intra-type Förster resonance energy transfer in bulky size indoline sensitizer for dye-sensitized solar cells: A combined DFT/TDDFT and molecular dynamics study

Wei-Lu Ding, Quan-Song Li*, Ze-Sheng Li*

Beijing Key Laboratory of Photoelectronic/Electrophotonic Conversion Materials, Key Laboratory of Cluster Science of Ministry of Education, School of Chemistry, Beijing Key Laboratory for Chemical Power Source and Green Catalysis, School of Chemistry, Beijing Institute of Technology, Beijing 100081, China

Table S1. The vertical excited energies calculated by different functionals in CH_2Cl_2 solution.

Sensitizer	BHandHLYP	CAM-B3LYP	PBE0	MPW1K	Exp.[a]
IQ4	2.57/482	2.61/474	1.89/657	2.34/529	2.35/526

[a] Data from ref.44.

Table S2. The most relevant geometrical parameters of isolated and aggregate structures on TiO_2 film (unit in Å).

Adsorbed system		C-O_{S1}	C-O_{S2}	O_{S2}···H	H···O_{Ti}[a]	Ti_1-O_{S1}	Ti_2-O_{S2}
IQ4-monomer@TiO_2		1.298	1.280	/	/	2.024	2.136
-aggregate@TiO_2	(1,1)	1.299 [a]	1.273 [a]	/	/	2.031 [a]	2.106 [a]
		1.288 [a]	1.280 [a]	/	/	2.014 [a]	2.118 [a]
		1.298 [b]	1.272 [b]	/	/	2.022 [b]	2.106 [b]
		1.289 [b]	1.278 [b]	/	/	2.010 [b]	2.117 [b]
	(-1,1)	1.290 [a]	1.274 [a]	/	/	2.068 [a]	2.106 [a]
		1.293 [a]	1.279 [a]	/	/	2.103 [a]	2.103 [a]
		1.293 [b]	1.274 [b]	/	/	2.029 [b]	2.106 [b]
		1.296 [b]	1.275 [b]	/	/	2.022 [b]	2.103 [b]
	(3,1)	1.301 [a]	1.269 [a]	/	/	2.021 [a]	2.116 [a]
		1.289 [a]	1.277 [a]	/	/	2.025 [a]	2.116 [a]
		1.298 [b]	1.271 [b]	/	/	2.019 [b]	2.107 [b]
		1.288 [b]	1.277 [b]	/	/	2.017 [b]	2.119 [b]
	(-3,1)	1.292 [a]	1.275 [a]	/	/	2.030 [a]	2.099 [a]
		1.279 [a]	1.298 [a]	/	/	2.144 [a]	2.108 [a]
		1.290 [b]	1.277 [b]	/	/	2.024 [b]	2.095 [b]
		1.278 [b]	1.299 [b]	/	/	2.137 [b]	2.106 [b]
YA421-monomer@TiO_2		1.298	1.281	/	/	2.023	2.135
-aggregate@TiO_2	(1,1)	1.253 [a]	1.338 [a]	1.012 [a]	1.760 [a]	2.221 [a]	/
		1.289 [a]	1.281 [a]	1.312 [a]	1.091 [a]	2.107 [a]	/
		1.334 [b]	1.248 [b]	1.756 [b]	0.991 [b]	2.014 [b]	/
		1.308 [b]	1.265 [b]	1.489 [b]	1.030 [b]	2.019 [b]	/
	(0,2)	1.308 [a]	1.269 [a]	1.498 [a]	1.009 [a]	2.026 [a]	/
		1.269 [a]	1.307 [a]	1.173 [a]	1.206 [a]	2.127 [a]	/
		1.310 [b]	1.267 [b]	1.550 [b]	0.999 [b]	2.016 [b]	/
		1.227 [b]	1.368 [b]	0.994 [b]	1.971 [b]	2.892 [b]	/
	(2,2)	1.289 [a]	1.283 [a]	1.322 [a]	1.082 [a]	2.107 [a]	3.250 [a]
		1.284 [a]	1.287 [a]	1.314 [a]	1.096 [a]	2.101 [a]	3.295 [a]
		1.316 [b]	1.260 [b]	1.720 [b]	0.983 [b]	2.021 [b]	/
		1.290 [b]	1.282 [b]	1.373 [b]	1.070 [b]	2.107 [b]	/
YA422-monomer@TiO_2		1.293 [a]	1.285 [a]	/	/	2.109 [a]	2.127 [a]
-aggregate@TiO_2	(0,2)	1.309 [a]	1.269 [a]	1.511 [a]	1.006 [a]	2.022 [a]	2.901 [a]
		1.265 [a]	1.312 [a]	1.150 [a]	1.234 [a]	2.151 [a]	3.195 [a]
		1.314 [b]	1.260 [b]	1.736 [b]	0.983 [b]	2.021 [b]	/
		1.270 [b]	1.303 [b]	1.203 [b]	1.179 [b]	2.141 [b]	/
	(2,2)	1.314 [a]	1.261 [a]	1.714 [a]	0.982 [a]	2.022 [a]	3.744 [a]
		1.304 [a]	1.271 [a]	1.451 [a]	1.029 [a]	2.021 [a]	3.120 [a]
		1.317 [b]	1.260 [b]	1.730 [b]	0.982 [b]	2.021 [b]	/
		1.310 [b]	1.266 [b]	1.521 [b]	1.017 [b]	2.014 [b]	/

[a] Before the CDCA co-adsorption

[b] After the CDCA co-adsorption