

Supplementary information for:

Calculations of the Light Absorption Spectra of Porphyrinoid Chromophores for Dye-Sensitized Solar Cells

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- 1) UV/Vis spectra calculated with the TDDFT (B3LYP, CAM-B3LYP and BHLYP), CC2 and ADC(2) methods, for the different systems studied in this work. The density functional or ab-initio method is indicated for each table. All systems calculated with the def2-SVPD basis set, COSMO solvation model (epsilon = 24), absence of TiO₂ cluster and the RIJONX (for CAM-B3LYP) or RIJCOSX (for B3LYP and BHLYP) approximations unless otherwise noted,

ZnPBA-H

CAM-B3LYP			CAM-B3LYP	No RIJONX		BHLYP	
wavelength/nm	oscillator str.		wavelength/nm	oscillator str.		wavelength/nm	oscillator str.
609.4	0.332		609.5	0.333		594.5	0.320
582.8	0.022		582.8	0.022		570.1	0.012
491.6	0.070		491.9	0.070		487.3	0.066
462.7	0.210		462.8	0.210		454.2	0.211
450.4	0.106		450.5	0.105		449.8	0.139
429.7	0.225		429.9	0.225		432.5	0.213
370.1	2.807		370.1	2.808		368	2.869
340.4	1.235		340.4	1.235		347.9	0.001
328.6	0.003		328.6	0.003		337.5	1.242
324.1	0.050		324.1	0.050		328.4	0.084

CAM-B3LYP	def2-TZVP		BHLYP	Vacuum		BHLYP	def2-TZVP
wavelength/nm	oscillator str.		Wavelength/nm	Osc. Strength		Wavelength/nm	Osc. Strength
608.6	0.317		586.5	0.302		594.2	0.305
583	0.019		567	0.009		570.8	0.009
490.7	0.075		448.7	0.084		486.4	0.069
462.4	0.219		430.3	0.260		454	0.220
450.4	0.116		416.7	0.176		449.9	0.153
430.2	0.227		393.5	0.247		432.8	0.213
370.3	2.799		367.6	2.857		368.1	2.872
341	1.227		337.1	1.204		338.1	1.235
326.5	0.005		322.7	0.056		327.4	0.056
323	0.033		305.2	0.002		347.2	0.001

B3LYP	No RIJCOSX		B3LYP	
Wavelength/nm	Oscillator str.		Wavelength/nm	Oscillator str.
780.5	0.298		780	0.298
728	0.064		727.2	0.065
691.4	0.081		691	0.081
636	0.034		635.6	0.034
526.5	0.040		526.4	0.040
525.7	0.097		525.6	0.097
515.9	0.181		515.8	0.182
478.1	0.030		474.3	0.036
454.4	0.204		452.3	0.200
407.1	1.783		407.1	1.782

ADC(2)	def2-TZVP/Vacuum		CC2	def2-TZVP/Vacuum		ADC(2)	def2-TZVP
wavelength /nm	Oscillator str.		Wavelength h/nm	Oscillator str.		Wavelength /nm	Oscillator str.
638.6	0.169		620.6	0.165		647.2	0.217
615	0.007		602.1	0.008		617.5	0.008
462.6	0.163		451.9	0.200		472.4	0.224
447.8	0.424		439.2	0.403		456.8	0.621
435	0.510		430.1	0.483		442.6	0.666
417.8	0.150		413.4	0.085		423.6	0.151
386.4	2.051		380.2	1.737		397.6	1.902
369.8	0.875		363.7	0.672			
353.4	0.005		352.8	0.021			
334.2	0.070		330.9	0.021			

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CAM-B3LYP			CAM-B3LYP	TiO2 cluster		CAM-B3LYP	Vacuum
Wavelength/n m	Oscillator str.		Wavelength/nm	Oscillator str.		Wavelength/nm	Oscillator str.
601.7	0.285		603.4	0.327		597.2	0.398
582.4	0.030		582.6	0.029		594.5	0.057
480.8	0.070		481.5	0.069		542.5	0.000
461.9	0.203		461.7	0.204		473.1	0.000
447.7	0.071		447.8	0.075		472.2	0.000
428.8	0.193		428.4	0.197		466.9	0.000
368.7	2.665		422.8	0.004		423	0.000
345.3	1.285		374.4	0.000		420.8	0.646
325.9	0.006		371.1	3.084		415.4	0.470
321.9	0.017		344.5	1.231		415.2	0.000

BHLYP			BHLYP	TiO2 cluster		BHLYP	Vacuum
Wavelength/nm	Osc. Strength		Wavelength/nm	Osc. Strength		Wavelength/nm	Osc. Strength
586.9	0.270		588.4	0.308		585.3	0.078
569.8	0.018		569.9	0.018		585	0.367
474.9	0.068		475.9	0.067		472.5	0.000
453.7	0.212		453.5	0.213		458.3	0.000
446.4	0.086		446.6	0.092		429.9	0.000
430.4	0.185		430.2	0.187		427.4	0.000
367.3	2.711		368.9	3.089		423.7	0.000
344.7	1.274		343.5	1.260		419.2	1.027
339.3	0.002		357.6	0.000		409.6	0.102
309.6	0.062		313.6	0.045		395.4	0.540

BHLYP	TiO2/Vacuum		CAM-B3LYP	TiO2/Vacuum	BHHLYP	TiO2(2)
Wavelength/nm	Osc. strength		Wavelength/nm	Osc. strength	Wavelength/nm	Osc. strength
580.2	0.353		593.5	0.367	588	0.318
574.6	0.032		585.6	0.042	567.7	0.012
425.3	0		446.9	0.002	479.4	0.069
410.8	0.274		420.7	0.249	453.3	0.212
405.3	0.118		420.3	0.006	448.9	0.110
398.3	0		412.4	0.001	446.8	0.000
397.7	1.158		398.9	1.682	430.2	0.192
390	1.181		395.5	0.001	413.6	0.000
384.9	0.002		391.6	0.014	406.5	0.000
374.8	0.325		391.4	0.851	368.3	3.193

BHHLYP	TiO2(2)(Vacuum)
Wavelength/nm	Osc. strength
576.8	0.304
568.1	0.021
413.3	0.279
410.3	0.092
398.3	0.017
382.4	2.702
373	0.242
357.2	0.852
333.4	0.001
333	0.002

ADC(2)	def2-TZVP/Vacuum		CC2	def2-TZVP/Vacuum		ADC(2)	def2-TZVP
Wavelength/nm	Oscillator str.		Wavelength/nm	Oscillator str.		Wavelength/nm	Oscillator str.
630.7	0.187		617.9	0.030		641	0.189
629.9	0.040		615.6	0.206		615.8	0.011
551.3	0.000		493.2	0.000		462.3	0.295
484	0.000		444.6	0.000		451.9	0.698
476.3	0.000		439.6	0.000		441.5	0.578
472.4	0.000		431.8	0.000		422.5	0.144
427.1	1.435		429.5	1.358		395.7	1.834
426.8	0.058		415.7	0.718			
422.4	0.000		410.3	0.435			
420.9	0.736		403.6	0.179			

ZNPBA-

CAM-B3LYP			CAM-B3LYP	TiO2 cluster
wavelength/nm	oscillator str.		wavelength/nm	oscillator str.
569.4	0.060		569.9	0.063
567	0.051		567.6	0.053
453.9	0.184		452.2	0.203
453.7	0.192		451.1	0.186
412.4	0.164		424	0.002
409.9	0.232		413.6	0.183
327	0.037		411.2	0.236
326.8	2.031		374.8	0.000
323.3	1.751		358.2	0.024
316.8	0.055		342.9	0.018

BHLYP			BHLYP	TiO2 Cluster
Wavelength/nm	Osc. Strength		Wavelength/nm	Osc. Strength
555.5	0.045		556	0.048
553.8	0.038		554.4	0.039
445	0.205		440.5	0.190
444.7	0.187		442.4	0.215
411.5	0.173		412.7	0.193
409.5	0.231		410.9	0.235
322.1	2.220		359.5	0.002
318.7	1.901		322.4	2.488
331.9	0.064		318.1	1.828
293.7	0.064		331.6	0.082

2) Cartesian coordinates (in Angstroms) for the optimized geometries of the systems studied in this work.

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Zn	4.00954945587326	15.84796904316489	7.04929045621929
O	-2.04621098206542	6.92928492353911	0.52693012957859
O	-2.53914315563533	6.17485304308901	2.60589963609815
C	2.91524101294379	14.24288876844649	4.63844369527718
C	2.95485966852663	14.18091734738281	3.19014516366094
C	3.69681042191965	15.26020134664325	2.76597894125824
C	4.09621719676497	15.98303208125672	3.95736411170541
C	2.65349511844504	13.87154473308865	9.00098656238118
C	1.84000525741665	12.66995675347941	9.03722784312062
C	1.60291273631055	12.30918812085336	7.73049019469616
C	2.27071095228567	13.29316260043707	6.89899549718316
C	5.10402659987870	17.45927507261738	9.45344938950050
C	5.04044511410281	17.54079259600107	10.90042066963349
C	4.29966090467565	16.45989118613857	11.32293081064401
C	3.90425726481524	15.72786695985699	10.13354576030325
C	5.36241391154050	17.84060931632323	5.10301935975382
C	6.18014100341871	19.03795782500822	5.06891500001500
C	6.44266127650996	19.37529091312581	6.37765227754367
C	5.76161017077993	18.39832726171159	7.20556798160281
C	5.75777019794315	18.40474577440010	8.62292590756864
C	4.89092293813034	17.15305142185476	3.95518254983048
C	3.10106850947903	14.56165627631866	10.14798457951076
C	2.26604865325467	13.27924447820631	5.46992568792709
C	2.67529782923948	14.03300053045084	11.48679911470644
C	1.43758482733438	14.44861230919914	12.04405643949287
C	1.05308664995602	13.93934682961362	13.29920172106582
C	1.86298481283558	13.03280325170608	14.01473015037452
C	3.08608394296059	12.63725192601047	13.43787276369523
C	3.50954434330919	13.12320678081761	12.18393122845014
C	1.56882683856557	12.22133105034874	4.82941525249673
C	0.95203957233740	11.30220329172164	4.28046215222227

C	0.23224018748669	10.24560278724485	3.66159099378237
C	-0.42466232894088	9.26020859799614	4.45352850631899
C	-1.13510969469109	8.22144188667056	3.84688346961037
C	-1.21080521882295	8.13428259072567	2.43679512227408
C	-0.56037788719058	9.10871324330406	1.64500497719746
C	0.15167534903203	10.15058084691757	2.24180451860698
C	-1.95769083146943	7.04314859321708	1.74543553582575
C	7.61931984332614	19.14897018908335	10.02891602134994
C	8.44900216648069	18.07581727863027	9.63351589530381
C	9.57068873229651	17.72522418872497	10.40056501805281
C	9.91807597733056	18.43296635631265	11.57116922786273
C	9.08018127837447	19.50735186021536	11.95317405934641
C	7.94719778098057	19.85915560153919	11.20920580574477
C	5.96541800027567	20.78856193050578	9.15365184170441
C	4.57410006098188	21.01464988608821	9.05654622691806
C	4.07597255295938	22.31601443136637	8.89144970039561
C	4.93387731615065	23.43550405075935	8.83547145595616
C	6.32446824782617	23.19444102858451	8.93578167425562
C	6.83919806309297	21.90028810326462	9.08259916405976
C	11.14058921949262	18.07607318564646	12.38470565252273
C	4.39732027241771	24.84135571352622	8.69652070353415
C	6.61619974704967	17.61314003937357	2.27741952062883
C	7.20652531711650	18.62306492376393	1.47927168468266
C	7.42590204026544	16.54001818360818	2.71467276515385
C	8.55829987623193	18.54157176476202	1.12172883627547
C	8.78280168665292	16.48343918688473	2.36191879851229
C	9.38021277066330	17.47378579998456	1.55275946572268
C	4.24795213408258	18.26689178773677	1.87167432304867
C	3.16852720707394	18.95097244172242	2.47556545162676
C	4.26539678981788	18.14016292495862	0.46232760762085
C	2.14080588697941	19.49116224324285	1.68842359694755
C	3.24022543517161	18.70138529286928	-0.31058301861049
C	2.15459162331019	19.38887534682937	0.28005473997142
C	10.83173365826921	17.39332551761221	1.14027366139211
C	1.06971228029217	20.01318966565390	-0.56671757497891
C	4.82517741396169	12.68393937607913	11.58321078156566
C	0.55654682551050	15.42245584581873	11.29612463079413
C	1.43605039277353	12.52552237751939	15.37374059177680
N	3.60810352057061	15.34536154767362	5.08502528473805
N	2.90247080853076	14.22851737573442	7.68403149006047
N	4.41019034512431	16.35264929079345	9.00905140985948
N	5.11635944773561	17.47215973374965	6.40965631359382
N	6.46145283777645	19.46487496329726	9.27299789817644

N	5.25929148294286	17.68592054680614	2.67972704802258
H	2.48462482268167	13.40201694827638	2.57898739514636
H	3.95034401872125	15.54159821688804	1.73815519286601
H	1.49865175068415	12.17051794306945	9.95127337657293
H	1.02602865337518	11.45536534554310	7.35711237459669
H	5.50317143008048	18.32180504523974	11.51349637969154
H	4.03130502473298	16.18285740298941	12.34896310292119
H	6.52257857677761	19.54849129771408	4.16240374047807
H	7.03527094753554	20.21900533312570	6.74711485712125
H	-0.36825066672347	9.32389083065599	5.55023609583472
H	-1.63841863054654	7.46714956232123	4.46787411866285
H	-0.62582594636812	9.03145058045096	0.54948420368369
H	0.65507651664452	10.90574956598433	1.62031092223654
H	8.20779586620578	17.51049173341529	8.72092468960821
H	10.19812826473848	16.88150486869765	10.07009416174534
H	9.31144014231349	20.07416059817733	12.87000374754754
H	7.30220166636222	20.68326639716536	11.54795414357529
H	3.88142209736103	20.16137107477338	9.10644731265481
H	2.98640821357773	22.46336016163907	8.81441584481286
H	7.02567341214009	24.04319584146518	8.87952608366781
H	7.92694584523984	21.74376951813621	9.13125898134223
H	11.57509467496425	17.10730491909390	12.06834864577852
H	10.90200725199214	18.01038007674760	13.46696042039713
H	4.99610711922044	25.43577145812051	7.97559223346168
H	3.34244891454980	24.84631714065612	8.35736300933370
H	3.73248642252940	11.92584683427737	13.97855877338127
H	0.09077553505150	14.26036187334443	13.73218315748365
H	11.93262000751087	18.84916531527101	12.27929870214940
H	4.43734364996783	25.38178415559805	9.66763536942027
H	6.60287446039798	19.48091053694448	1.14847763632917
H	6.98688183522779	15.74901725396760	3.34069730725537
H	8.99344058126565	19.34303998837363	0.50225892802396
H	9.39064672745862	15.63692055793688	2.72094629950916
H	3.13641110513432	19.05347762727823	3.57052477814465
H	5.08234004062143	17.58817256858245	-0.02546533604652
H	1.30885434565094	20.01615059400136	2.18557201646432
H	3.27534908253507	18.58582415596871	-1.40633394420097
H	11.32231971132338	18.38784069223643	1.18086100826003
H	11.40377021625092	16.69869098934266	1.78704035923038
H	10.93125685297715	17.02969090867036	0.09388740648526
H	0.11843748763508	20.11181126114309	-0.00618721887495
H	1.36107347824526	21.03399878777639	-0.89932844119552
H	0.87357922714424	19.41960971843058	-1.48290446322954

H	4.67237491357327	12.19780205760769	10.59658586103270
H	5.49084383585154	13.55386807717490	11.40102607496692
H	5.35817691135028	11.97138854703318	12.24211875603273
H	1.09518477963355	16.37215728567619	11.09394492292954
H	0.26091055417015	15.01607267807573	10.30614195751693
H	-0.36444721872303	15.66028361573910	11.86271116799183
H	0.35302603984196	12.28629249344650	15.39652843059915
H	1.99916135432485	11.61829066881121	15.66974506783157
H	1.61119659538519	13.29570901034029	16.15631127260717
H	-3.00374015774094	5.49553754699655	2.06729121144456

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Zn	4.01062087835300	15.85071779197398	7.06206659811968
O	-2.01446609327219	7.04691601781267	0.41449882162975
O	-2.53841228563503	6.17096386387275	2.44256686780135
C	2.91902179802863	14.23567147518383	4.65557895496774
C	2.95959457517499	14.17093440326068	3.20812190414273
C	3.70144369845744	15.24984086587352	2.78140273653860
C	4.10052309844229	15.97492824719898	3.97113351890954
C	2.65357483083602	13.88028860598628	9.01731543958682
C	1.84038951954742	12.67910790791187	9.05689878036349
C	1.60440202758696	12.31392338481342	7.75056472580792
C	2.27242310985820	13.29412893461173	6.91650611565741
C	5.10194880732641	17.47042507545627	9.46116063590055
C	5.04322823933394	17.55306915659855	10.90865486403683
C	4.30239786807675	16.47355394624486	11.33443694462435
C	3.90255365628315	15.73995082028083	10.14698358449222
C	5.36499378445321	17.83725567689380	5.11026146833152
C	6.18119613588089	19.03596393019201	5.07376181673890
C	6.44208243103785	19.37746096394341	6.38179413616828
C	5.76280754789022	18.40070814866307	7.21218600501685
C	5.75644799135736	18.41238936625642	8.62866695597160
C	4.89558508346399	17.14612411509489	3.96598538935060
C	3.10053825415245	14.57470777745748	10.16402496989507
C	2.26792465841646	13.27384274872445	5.48757473521564
C	2.67369820210954	14.04901587597310	11.50373653196519
C	1.43509329793898	14.46488754858162	12.05884178130260
C	1.04935888093061	13.95858252963227	13.31486671709166

C 1.85900660094789	13.05444013563620	14.03365293837537
C 3.08291814573712	12.65813336014330	13.45904020604124
C 3.50729014722602	13.14115837509071	12.20423432124616
C 1.57061902279536	12.21451372299617	4.84706647217200
C 0.95435254016884	11.29937754607233	4.29059860011806
C 0.23505265165485	10.25151327310878	3.65131249786712
C -0.41486582031598	9.24300824024147	4.41982998447462
C -1.12181606126245	8.21799347207529	3.78138172965243
C -1.20784685495693	8.15726361636331	2.37354419057918
C -0.56318983337820	9.15635662582436	1.61250348263840
C 0.14900521049440	10.19039636496239	2.23043682644176
C -1.99225483131954	7.02061309012617	1.67976878505225
C 7.63062615540029	19.16554391436300	10.01309078144224
C 8.45862891278861	18.09524358779088	9.60561360909995
C 9.59394061730269	17.74943899193085	10.35472827216160
C 9.95709724250601	18.45797616315175	11.52000620595220
C 9.12014834349905	19.52805922987431	11.91561672800033
C 7.97427889909884	19.87546793784869	11.18940185498004
C 5.94940211728195	20.79504168033687	9.16989981517201
C 4.55512547104421	21.00829472594545	9.08295034604190
C 4.04262209524734	22.30547209405314	8.92871246628366
C 4.88819329038814	23.43426065884974	8.87256534468201
C 6.28173632323112	23.20649704079049	8.96102793383039
C 6.81058966775541	21.91683392858972	9.09749128533265
C 11.19366429235529	18.10572375151540	12.31438728255185
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C 6.62181369125817	17.58778562114007	2.28361343550598
C 7.21926341016836	18.58927296565776	1.47994300793018
C 7.42438652464560	16.51065370282900	2.72451909035545
C 8.56968330045447	18.49533946027715	1.12000669160193
C 8.77997804945099	16.44143197332289	2.36907680065381
C 9.38387211678591	17.42295043208884	1.55391331236851
C 4.25811908637473	18.25952985548090	1.88088655601955
C 3.18126061623963	18.94744230093285	2.48555806420887
C 4.27317826748884	18.13325405762829	0.47121987492979
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C 2.16702319565472	19.39029483680601	0.29101601410471
C 10.83384678768181	17.32859248375423	1.13852873829733
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ZnPBAT--TiO2

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H	1.54282643092586	12.15040570410975	9.97918394347504
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O	-7.69799998894850	1.65199999932559	-1.36000003027649
O	-4.11700000420533	1.10999999755132	-2.05799998162095
O	-1.96100000632956	4.32500006812440	0.85200003082752

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ZnPBAT--TiO2(2)

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ZnPBA--TiO2

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