

Electronic Support Information

Improved Charge Transfer Performance of Eosin Y-Sensitized Anatase TiO₂ by Anchoring Group Modification: from the Theory to Experiment

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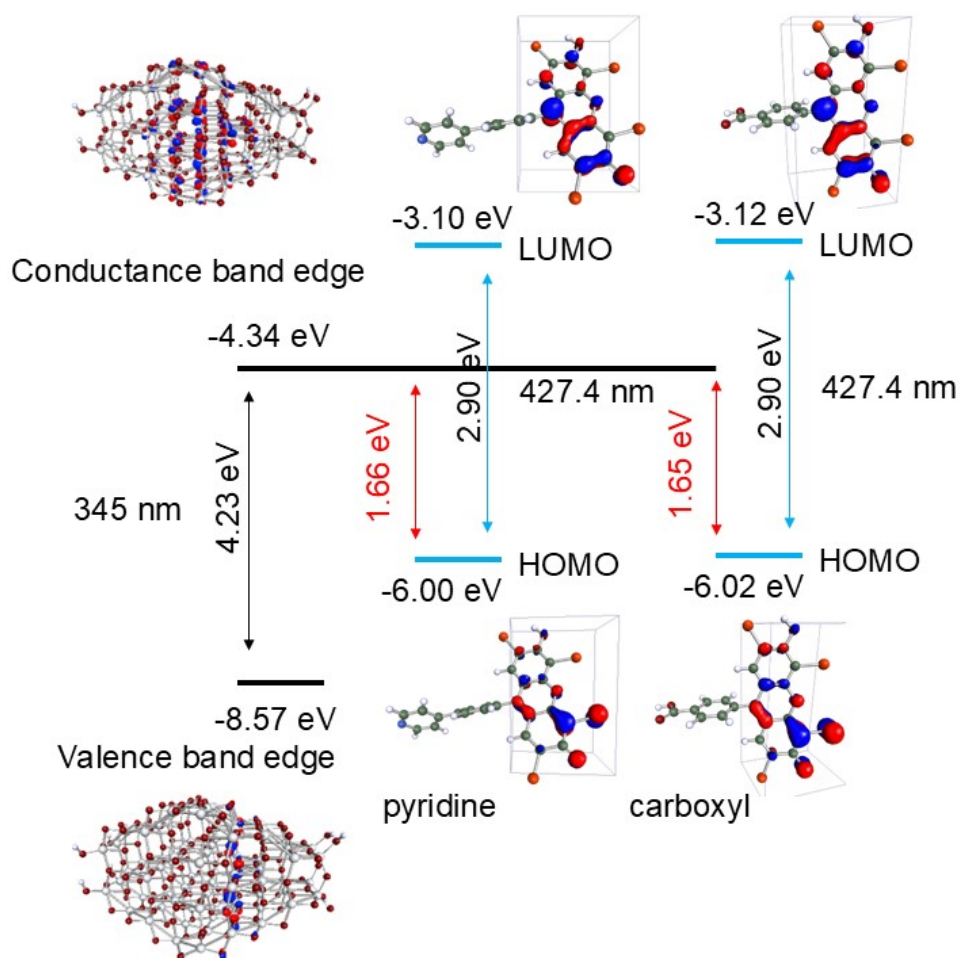
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Figure S1: Alignment of the valence and conduction band edges of TiO₂ nanoparticle with eosin Y pyridine and carboxyl derivatives HOMO and LUMO.

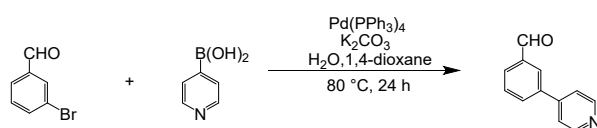


Synthesis of Eosin Y derivatives

General Information

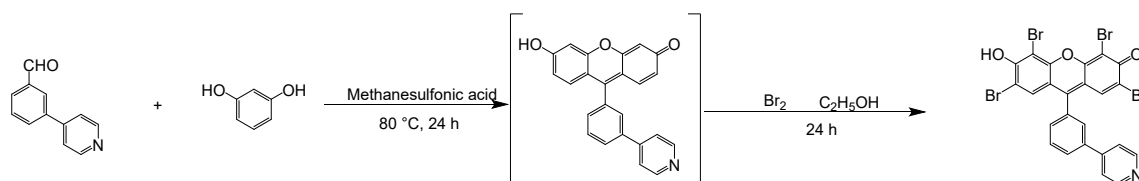
The ¹H spectrum was recorded on a Bruker AV600 (600 MHz) spectrometer. The ¹H NMR chemical shifts were reported to be δ values (ppm) relative to Me₄Si. The absorption spectra were recorded on a Shimadzu UV-3600. All the solvents and reagents were of reagent quality, purchased commercially, and used without further purification.

Synthesis of 3-(pyridin-4-yl)benzaldehyde



Under a nitrogen atmosphere, a solution of 3-bromobenzaldehyde (1.6 g, 8.6 mmol), pyridin-4-ylboronic acid (2.0 g, 16.3 mmol), tetrakis(triphenylphosphine)palladium(0) (0.6 g, 0.5 mmol) and Potassium carbonate (7.5 g, 54.0 mmol) was dissolved in H₂O (7.5 mL) and 1,4-dioxane (75 mL). The solution was heated at 80 °C for 24 h. After the reaction, the mixture was concentrated in vacuo. The crude product was purified by a silica gel chromatograph eluted with hexane : ethyl acetate (2:1) to give compound (1.5 g, 94 %) as white solids.

¹H NMR (600 MHz, CDCl₃) 7.55 (d, J=4.8 Hz, 2H), 7.68 (d, J=7.6 Hz, 1H), 7.91 (d, J=7.6 Hz, 1H), 7.95 (d, J=7.5 Hz, 1H), 8.15 (s, 1H), 8.71 (d, J=4.7 Hz, 2H), 10.11 (s, 1H).

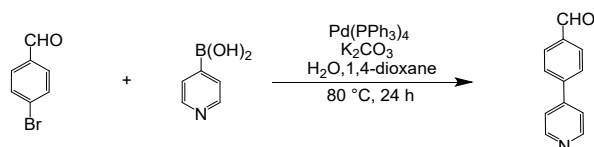


Synthesis of 2,4,5,7-tetrabromo-6-hydroxy-9-(3-(pyridin-4-yl)phenyl)-3H-xanthen-3-one (MPyE)

Under a nitrogen atmosphere, a solution of 3-(pyridin-4-yl) benzaldehyde (1.5 g, 8.2 mmol), resorcinol (1.8 g, 16.4 mmol) was dissolved in methanesulfonic acid (25 mL). The solution was heated at 80 °C for 24 h. After the reaction, the mixture was added in 3M sodium acetate solution. Then, filtered the solid and washed with 100 mL of ion-exchanged water, and the solid compound was collected and it was used as a source of the following reaction. A mixture of (0.9 g, 2.5 mmol), ethanol (125 mL) was dropped bromine (2.4, 15 mmol, 6 equiv.) at room temperature, then stirred overnight. After reaction, the precipitated crystal was corrected, washed with ethanol, gave compound as red powder (0.6 g, 36 %).

¹H NMR (600 MHz, DMSO-*d*₆) 7.29 (s, 1H), 7.77 (d, J=7.8 Hz, 2H), 8.32 (d, J=7.8 Hz, 2H), 8.51-8.57 (m, 2H), 8.88-8.96 (m, 2H), 9.01-9.08 (m, 2H).

Synthesis of 4-(pyridin-4-yl)benzaldehyde

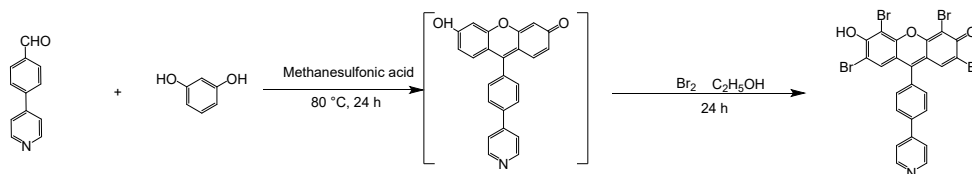


Under a nitrogen atmosphere, a solution of 3-bromobenzaldehyde (1.6 g, 8.6 mmol), pyridin-4-ylboronic acid (2.0 g, 16.3 mmol), Tetrakis(triphenylphosphine)palladium(0) (0.6 g, 0.5 mmol) and Potassium carbonate (7.5 g, 54.0 mmol) was dissolved in H₂O (7.5 mL) and 1,4-

dioxane (75 mL). The solution was heated at 80 °C for 24 h. After the reaction, the mixture was concentrated in vacuo. The crude product was purified by a silica gel chromatograph eluted with hexane : ethyl acetate (2:1) to give compound (1.0 g, 63 %) as white solids.

¹H NMR (600 MHz, CDCl₃) 7.56 (dd, J=2.9, 6.1 Hz, 2H), 7.82 (d, J=8.2 Hz, 2H), 8.03 (d, J=8.2 Hz, 2H), 8.74 (d, J=5.8 Hz, 2H), 10.11 (s, 1H).

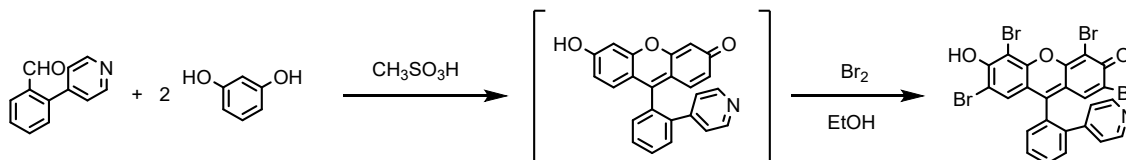
Synthesis of 2,4,5,7-tetrabromo-6-hydroxy-9-(4-(pyridin-4-yl)phenyl)-3H-xanthen-3-one (PPyE)



Under a nitrogen atmosphere, a solution of 3-(pyridin-4-yl) benzaldehyde (1.5 g, 8.2 mmol), resorcinol (1.8 g, 16.4 mmol) was dissolved in methanesulfonic acid (25 mL). The solution was heated at 80 °C for 24 h. After the reaction, the mixture was added in 3M sodium acetate solution. Then, filtered the solid and washed with 100 mL of ion-exchanged water, and the solid compound was collected, and it was used as a source of the following reaction. A mixture of (0.9 g, 2.5 mmol), ethanol (125 mL) was dropped bromine (2.4, 15 mmol, 6 equiv.) at room temperature, then stirred overnight. After reaction, the precipitated crystal was corrected, washed with ethanol, gave compound as red powder (0.7 g, 42 %).

¹H NMR (600 MHz, DMSO-*d*₆) 7.23 (s, 1H), 7.74 (d, J=5.2 Hz, 2H), 7.88-7.94 (m, 2H), 8.18 (s, 1H), 8.31 (d, J=5.2 Hz, 1H), 8.41-8.46 (m, 2H), 8.94-9.01 (m, 2H).

Synthesis of 2,4,5,7-tetrabromo-6-hydroxy-9-(2-(pyridin-4-yl)phenyl)-3H-xanthen-3-one (OPyE)

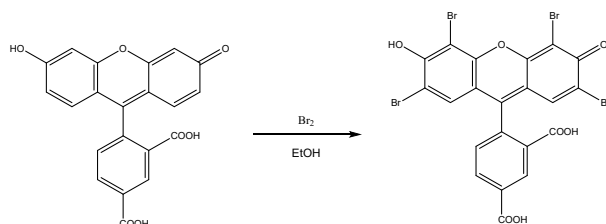


Under a nitrogen atmosphere, a solution of 2-(pyridin-4-yl)benzaldehyde (500 mg, 2.74 mmol), resorcinol (600 mg, 5.47 mmol) was dissolved in methanesulfonic acid (10 mL). The solution was heated at 80 °C for 24 h. After the reaction, the mixture was added in 3M sodium acetate solution. Then, filtered the solid and washed with 200 mL of ion-exchanged water, and the solid compound was collected and it was used as a source of the following reaction. A mixture of (900 mg, 2.47 mmol), ethanol (90 mL) was dropped bromine (5.4 g, 30 mmol, 12.2 equiv.) at

room temperature, then stirred overnight. After reaction, the precipitated crystal was corrected, washed with ethanol, gave compound as red powder (678 mg, 40 %).

^1H NMR (400MHz, DMSO- d_6), 8.67 (brs, 2H), 7.91-7.78 (m, 3H), 7.69-7.57 (m, 3H), 7.19 (s, 2H)

Synthesis of 4-(2,4,5,7-tetrabromo-6-hydroxy-3-oxo-3H-xanthen-9-yl)isophthalic acid (PEY)



A mixture of 5-carboxyfluorescein [1] (1.12 g, 2.99 mmol), ethanol (30 mL) was dropped bromine (0.9 mL, 16.89 mmol, 5.6 equiv.) at room temperature, then stirred over night. After reaction, the precipitated crystal was corrected, washed with ethanol, gave compound as red micro-crystalline powder (400 mg, 19%).

^1H NMR (400 MHz, DMSO- d_6) δ = 8.65 (s, 1H), 8.35 (d, J = 8.9 Hz, 1H), 7.65 (d, J = 7.8 Hz, 1H), 7.03 (s, 2H)

[1] Y. Ueno, G.-S. Jiao, K. Burgess, Synthesis 2004, 15, 2591-2593.

Table S1. Cartesian coordinates of the optimized geometry of orto-Eosin Y and anatase cluster.

All coordinates are in angstroms.

1	O	21.6711	13.9247	23.3356
2	O	21.5563	13.9593	32.746
3	O	21.6033	21.8133	23.307
4	O	13.9624	13.8502	23.29
5	O	14.2511	22.0601	23.459
6	O	21.6226	17.7663	23.3331
7	O	21.5039	17.5753	32.7808
8	O	21.7053	9.706	23.302

9	O	13.9295	17.5962	23.2639
10	O	14.0857	10.0214	23.3903
11	O	25.4834	14.0401	23.4932
12	O	25.3525	21.568	23.7027
13	O	17.8001	13.8724	23.2145
14	O	17.6998	13.915	32.6722
15	O	17.7405	21.9404	23.3155
16	O	25.4392	17.8351	23.5955
17	O	25.2014	9.5986	23.5726
18	O	17.7502	17.7301	23.2793
19	O	17.6511	17.5368	32.6862
20	O	17.8396	9.8302	23.1475
21	O	19.6686	13.9711	24.8685
22	O	19.8856	13.9302	15.0507
23	O	19.5889	13.9449	34.3106
24	O	19.6737	21.9402	24.9433
25	O	19.6785	17.6461	24.9001
26	O	19.8706	17.8317	15.0796
27	O	19.5371	17.5173	34.335
28	O	19.7102	9.6746	24.8504
29	O	23.5071	13.9077	25.0664
30	O	23.3862	13.8161	34.4185
31	O	23.3234	22.018	25.1888
32	O	15.918	14.2541	24.8337
33	O	15.7484	13.8155	34.2257
34	O	15.9758	20.9712	24.9344
35	O	23.4203	17.3185	25.0125
36	O	23.3264	17.7162	34.464
37	O	23.4069	10.6222	25.0141
38	O	15.8288	17.7211	24.9347
39	O	15.6956	17.5892	34.236
40	O	16.049	9.6309	24.9708
41	Ti	21.5322	13.9763	25.3093
42	Ti	21.5667	13.9389	15.7652
43	Ti	21.5261	14.0449	34.8432

44	Ti	21.4843	21.4781	25.4345
45	Ti	14.152	13.9855	25.1025
46	Ti	14.1812	21.1634	25.1441
47	Ti	21.4869	17.6974	25.3432
48	Ti	21.5617	17.8805	15.7864
49	Ti	21.4748	17.4409	34.8788
50	Ti	21.5018	10.2818	25.3318
51	Ti	14.0099	17.617	25.108
52	Ti	14.3262	10.2934	25.2067
53	Ti	25.2967	13.9872	25.3298
54	Ti	25.0206	21.3163	25.4937
55	Ti	17.8251	13.9118	25.2385
56	Ti	18.1681	13.8696	15.694
57	Ti	17.5942	14.0086	34.7734
58	Ti	17.858	21.3278	25.3399
59	Ti	25.1405	17.648	25.386
60	Ti	25.1906	10.4452	25.2776
61	Ti	17.773	17.6428	25.2611
62	Ti	18.1618	17.8163	15.7294
63	Ti	17.548	17.4148	34.7929
64	Ti	17.8782	10.1378	25.2816
65	O	21.4838	15.8027	25.7286
66	O	21.6632	15.8969	16.2699
67	O	21.5134	15.7369	35.5493
68	O	13.5486	15.7893	25.5442
69	O	21.5825	19.661	25.628
70	O	21.7241	19.7387	16.3233
71	O	21.2281	12.0394	25.6425
72	O	21.7752	12.0799	16.2413
73	O	13.4907	19.4524	25.38
74	O	14.4836	12.0843	25.4364
75	O	25.8643	15.8285	25.7374
76	O	17.8378	15.807	25.6332
77	O	18.05	15.8488	16.1966
78	O	17.6022	15.711	35.4529

79	O	24.7757	19.5324	25.735
80	O	25.8474	12.1652	25.5696
81	O	18.1293	19.5692	25.6352
82	O	17.9486	19.6704	16.2231
83	O	17.7714	11.9488	25.4922
84	O	17.9992	12.0033	16.1956
85	O	21.6452	13.8802	27.3163
86	O	21.6576	13.9632	17.8663
87	O	21.4364	21.5879	27.269
88	O	13.5704	13.8136	27.1208
89	O	13.9025	21.4327	26.9435
90	O	21.6007	17.763	27.3127
91	O	21.6153	17.8098	17.8952
92	O	21.6383	10.0412	27.1313
93	O	13.6954	17.6806	27.2227
94	O	13.4486	10.3046	26.8916
95	O	25.6369	13.9054	27.429
96	O	25.9087	21.2712	27.1798
97	O	17.7758	13.8259	27.2
98	O	18.0387	13.9112	17.7963
99	O	17.6849	21.546	27.1404
100	O	25.7595	17.8019	27.3789
101	O	25.4559	10.1451	27.0796
102	O	17.7374	17.7051	27.2635
103	O	17.994	17.7604	17.8212
104	O	17.8994	10.0033	27.1166
105	Ti	21.6861	15.8002	27.7428
106	Ti	21.7862	15.8869	18.1759
107	Ti	13.9684	15.778	27.5997
108	Ti	21.5317	19.7626	27.7758
109	Ti	21.7088	19.6313	18.1259
110	Ti	21.5379	11.8772	27.7119
111	Ti	21.7751	12.1393	18.0597
112	Ti	14.0491	19.6252	27.6403
113	Ti	14.0243	11.9574	27.6107

114	Ti	25.5541	15.7889	27.9162
115	Ti	17.8255	15.7826	27.6576
116	Ti	17.8545	15.8309	18.0959
117	Ti	25.2839	19.6342	27.8898
118	Ti	25.284	11.928	27.8112
119	Ti	17.7893	19.7059	27.6998
120	Ti	17.8753	19.5826	18.0383
121	Ti	17.7885	11.8161	27.6487
122	Ti	17.9419	12.0849	17.9984
123	O	19.695	15.7863	27.9967
124	O	19.8121	15.8561	18.6312
125	O	19.6371	19.6227	28.1151
126	O	19.779	20.0464	18.5882
127	O	19.6749	11.9568	28.0566
128	O	19.8543	11.6634	18.5279
129	O	23.638	15.8711	28.0062
130	O	23.6247	15.9017	18.6543
131	O	15.7697	15.7145	27.834
132	O	16.0009	15.8105	18.4992
133	O	23.4241	19.7203	28.1113
134	O	23.5081	19.9015	18.7181
135	O	23.4828	12.0447	27.9342
136	O	23.5649	11.8587	18.6149
137	O	15.8471	19.5064	27.8378
138	O	16.0668	19.8626	18.523
139	O	15.8798	11.8797	27.8683
140	O	16.1233	11.8015	18.5104
141	O	21.6166	15.7822	29.665
142	O	21.7194	15.8535	20.3009
143	O	13.8003	15.7099	29.4348
144	O	21.5127	19.902	29.7932
145	O	21.6286	19.6516	20.362
146	O	21.594	11.6746	29.701
147	O	21.6944	12.1185	20.2787
148	O	13.9234	19.7686	29.453

149	O	13.9542	11.8274	29.4531
150	O	25.4988	15.8317	29.7371
151	O	17.705	15.7608	29.5844
152	O	17.8394	15.8375	20.2205
153	O	25.2969	19.7742	29.7426
154	O	25.3331	11.7641	29.6276
155	O	17.6572	19.8772	29.6958
156	O	17.8671	19.5712	20.2572
157	O	17.7322	11.6353	29.6548
158	O	17.9323	12.0299	20.2349
159	Ti	19.6292	15.7661	29.9973
160	Ti	19.7733	15.8405	20.5453
161	Ti	19.6001	19.5085	30.1772
162	Ti	19.7325	19.8675	20.5655
163	Ti	19.633	12.0244	30.1172
164	Ti	19.8183	11.8112	20.5081
165	Ti	23.6308	15.8054	30.1304
166	Ti	23.5219	15.854	20.4963
167	Ti	15.6136	15.7233	29.9398
168	Ti	16.0301	15.832	20.3453
169	Ti	23.477	19.5016	30.2543
170	Ti	23.4345	19.7488	20.5432
171	Ti	23.5201	12.0944	30.1827
172	Ti	23.4949	11.9658	20.4646
173	Ti	15.7129	19.4239	30.0761
174	Ti	16.0592	19.7272	20.373
175	Ti	15.7428	12.0465	30.0394
176	Ti	16.1187	11.9277	20.3403
177	O	19.6433	13.8295	30.2802
178	O	19.7724	13.8907	20.9202
179	O	19.6987	21.6865	21.048
180	O	19.6218	17.7015	30.3088
181	O	19.7581	17.7874	20.9519
182	O	19.8374	9.9872	20.9659
183	O	23.4915	13.9043	30.3598

184	O	23.9028	13.9454	20.905
185	O	23.7686	21.5432	21.1485
186	O	15.9002	13.8504	30.1909
187	O	15.6648	13.8669	20.7591
188	O	15.8257	21.5153	20.9272
189	O	23.4202	17.6965	30.4113
190	O	23.8723	17.8114	20.9625
191	O	23.7166	10.1689	21.0005
192	O	15.8269	17.6156	30.1944
193	O	15.632	17.736	20.7604
194	O	15.7682	10.1281	20.9024
195	O	19.6175	15.7531	31.9201
196	O	19.725	15.827	22.5636
197	O	19.5627	19.5593	32.0124
198	O	19.6554	19.7421	22.6749
199	O	19.6516	11.9445	31.9528
200	O	19.8074	11.9094	22.6188
201	O	23.7181	15.7922	32.1025
202	O	23.574	15.8473	22.5463
203	O	15.4255	15.7152	31.9137
204	O	15.8984	15.8107	22.3903
205	O	23.4982	19.564	32.0992
206	O	23.4291	19.6428	22.7755
207	O	23.5429	12.0096	32.0062
208	O	23.6264	12.0506	22.6253
209	O	15.5474	19.4445	31.8953
210	O	15.8236	19.6058	22.5175
211	O	15.6048	11.9956	31.8725
212	O	16.0049	12.0065	22.5702
213	Ti	19.6474	13.7957	32.4131
214	Ti	19.7188	13.9222	22.8469
215	Ti	19.7178	21.5519	22.8903
216	Ti	19.5916	17.699	32.4399
217	Ti	19.7059	17.7242	22.8772
218	Ti	19.7375	10.0957	22.8082

219	Ti	23.416	13.8325	32.5908
220	Ti	23.682	13.9474	22.9224
221	Ti	23.5596	21.4395	22.9598
222	Ti	15.8828	13.7982	32.4241
223	Ti	15.805	13.949	22.758
224	Ti	15.9047	21.4673	22.7833
225	Ti	23.3479	17.7377	32.6283
226	Ti	23.6241	17.6981	22.9553
227	Ti	23.5575	10.1858	22.8499
228	Ti	15.8343	17.6261	32.4389
229	Ti	15.7516	17.704	22.7815
230	Ti	15.8879	10.2021	22.7267
231	O	16.9355	14.1328	14.3915
232	O	16.8963	17.6672	14.4086
233	O	22.8703	14.1174	14.4849
234	O	22.8304	17.626	14.5173
235	H	16.6497	15.0323	14.1051
236	H	16.3697	18.4082	14.0419
237	H	23.4116	13.3851	14.1221
238	H	23.1107	16.7256	14.2266
239	O	17.8038	18.6598	36.0862
240	O	21.3241	12.7478	36.1306
241	O	17.8716	12.7521	36.0513
242	O	21.2245	18.706	36.1926
243	H	18.7087	18.9086	36.3941
244	H	22.0136	12.1054	36.4006
245	H	18.7786	12.496	36.3456
246	H	21.9178	19.3058	36.5388
247	C	32.7639	16.0453	28.1994
248	C	32.4038	16.0824	26.8424
249	C	31.0518	16.0332	26.4835
250	C	30.0482	15.9506	27.4732
251	C	30.4078	15.9115	28.8497
252	C	31.7735	15.9604	29.1913
253	C	29.3965	15.8492	29.9495

254	C	28.959	14.6286	30.4669
255	C	29.3572	13.3489	29.9365
256	C	28.8365	12.1821	30.4303
257	C	27.8698	12.1237	31.5705
258	C	27.4738	13.4572	32.0513
259	C	27.9875	14.6303	31.543
260	O	27.5667	15.8094	32.0797
261	C	27.9439	16.9982	31.5642
262	C	27.3804	18.1526	32.1297
263	C	27.6974	19.4326	31.6273
264	O	27.1352	20.5071	32.1815
265	C	28.6198	19.504	30.5406
266	C	29.1987	18.3671	29.9917
267	C	28.8736	17.0799	30.4913
268	Br	29.0218	21.2354	29.8573
269	Br	26.1473	17.987	33.5567
270	Br	26.2041	13.5177	33.4583
271	O	27.4571	11.0706	32.0506
272	Br	29.3194	10.5167	29.6886
273	C	28.6193	15.9023	27.0649
274	O	28.3786	15.9457	25.778
275	O	27.7103	15.8242	27.9224
276	H	33.8258	16.0825	28.4925
277	H	33.1789	16.1488	26.0621
278	H	30.7485	16.0584	25.4261
279	H	32.0589	15.9322	30.2551
280	H	30.0771	13.3261	29.1044
281	H	29.9079	18.4631	29.1566
282	H	27.3205	15.9023	25.6546

Table S2. Cartesian coordinates of the optimized geometry of meta-Eosin Y and anatase

cluster. All coordinates are in angstroms.

1	O	21.6458	13.8973	23.298
2	O	21.5378	13.909	32.6889
3	O	21.6438	21.7864	23.289
4	O	13.9364	13.884	23.3013
5	O	14.2926	22.0924	23.4833
6	O	21.6288	17.7408	23.304
7	O	21.5291	17.5417	32.7392
8	O	21.6441	9.6832	23.2599
9	O	13.9346	17.6358	23.2816
10	O	14.0294	10.0608	23.398
11	O	25.4599	13.9861	23.4245
12	O	25.3927	21.4978	23.6569
13	O	17.7737	13.8804	23.2025
14	O	17.6886	13.9156	32.6705
15	O	17.7828	21.9453	23.3211
16	O	25.4453	17.7724	23.5361
17	O	25.1514	9.5537	23.4986
18	O	17.7567	17.7356	23.2741
19	O	17.6794	17.5203	32.6875
20	O	17.7795	9.8365	23.1328
21	O	19.654	13.9505	24.8454
22	O	19.8058	13.9336	15.025
23	O	19.607	13.8976	34.2919
24	O	19.7259	21.9244	24.9371
25	O	19.6949	17.6372	24.8833
26	O	19.822	17.8359	15.06
27	O	19.5899	17.5025	34.3235
28	O	19.6597	9.6656	24.8231
29	O	23.4959	13.8789	25.0163
30	O	23.4275	13.8154	34.3105
31	O	23.3802	21.9675	25.1593
32	O	15.9043	14.2735	24.8338

33	O	15.7565	13.8313	34.2367
34	O	16.0186	20.9952	24.9508
35	O	23.4342	17.262	24.9677
36	O	23.4086	17.5836	34.3734
37	O	23.3697	10.556	24.9706
38	O	15.8456	17.7397	24.9415
39	O	15.7413	17.5859	34.2492
40	O	15.9976	9.6467	24.967
41	Ti	21.5224	13.9472	25.2715
42	Ti	21.4918	13.9277	15.7273
43	Ti	21.5584	13.9994	34.7908
44	Ti	21.537	21.4487	25.416
45	Ti	14.1383	14.0171	25.1117
46	Ti	14.2269	21.1979	25.1689
47	Ti	21.5078	17.6714	25.3129
48	Ti	21.5181	17.8707	15.7559
49	Ti	21.5438	17.3901	34.8323
50	Ti	21.4603	10.2495	25.2934
51	Ti	14.0273	17.6511	25.1242
52	Ti	14.2828	10.3244	25.2122
53	Ti	25.2907	13.9385	25.2598
54	Ti	25.0727	21.2474	25.4496
55	Ti	17.8122	13.9151	25.2257
56	Ti	18.0917	13.8856	15.6787
57	Ti	17.6092	13.9995	34.7718
58	Ti	17.9074	21.3299	25.3439
59	Ti	25.1604	17.5803	25.3286
60	Ti	25.1563	10.3857	25.2078
61	Ti	17.7918	17.6457	25.2556
62	Ti	18.1174	17.8324	15.7203
63	Ti	17.5972	17.4045	34.792
64	Ti	17.8328	10.1405	25.2647
65	O	21.4802	15.7734	25.693
66	O	21.606	15.8843	16.2347
67	O	21.5474	15.6848	35.5049

68	O	13.5531	15.8258	25.5586
69	O	21.6227	19.631	25.6062
70	O	21.6973	19.7264	16.2959
71	O	21.2125	12.0102	25.6055
72	O	21.6868	12.0655	16.2004
73	O	13.528	19.4908	25.4058
74	O	14.46	12.1136	25.4464
75	O	25.8894	15.7623	25.6818
76	O	17.8438	15.8082	25.6221
77	O	17.9934	15.8646	16.1862
78	O	17.6503	15.6994	35.451
79	O	24.806	19.4646	25.6882
80	O	25.8106	12.1062	25.4962
81	O	18.1628	19.5682	25.6324
82	O	17.9222	19.6868	16.2199
83	O	17.7375	11.9514	25.4784
84	O	17.9106	12.0197	16.1791
85	O	21.6405	13.8458	27.2773
86	O	21.5956	13.9475	17.8285
87	O	21.4976	21.5545	27.252
88	O	13.5595	13.8475	27.132
89	O	13.9595	21.4628	26.9723
90	O	21.6335	17.7294	27.2829
91	O	21.5844	17.7948	17.8641
92	O	21.5978	10.0089	27.0952
93	O	13.7199	17.7128	27.2417
94	O	13.4115	10.3443	26.9029
95	O	25.6458	13.8419	27.3644
96	O	25.9765	21.1818	27.1269
97	O	17.7682	13.8249	27.1878
98	O	17.976	13.9245	17.7827
99	O	17.7468	21.5435	27.1472
100	O	25.797	17.723	27.3147
101	O	25.4443	10.0893	27.0118
102	O	17.7626	17.7045	27.2577

103	O	17.9633	17.774	17.8143
104	O	17.8629	10.0048	27.1007
105	Ti	21.6958	15.7656	27.7006
106	Ti	21.741	15.87	18.1389
107	Ti	13.9766	15.8084	27.6109
108	Ti	21.5877	19.731	27.758
109	Ti	21.694	19.6154	18.098
110	Ti	21.519	11.8431	27.6752
111	Ti	21.6984	12.1223	18.0179
112	Ti	14.0958	19.6539	27.661
113	Ti	14.0036	11.9898	27.618
114	Ti	25.6008	15.7188	27.8546
115	Ti	17.8366	15.7808	27.6487
116	Ti	17.8098	15.8454	18.086
117	Ti	25.3407	19.5551	27.8361
118	Ti	25.2692	11.8695	27.7367
119	Ti	17.8379	19.7026	27.7012
120	Ti	17.8611	19.5969	18.0351
121	Ti	17.7651	11.8166	27.6343
122	Ti	17.8656	12.0988	17.9819
123	O	19.7058	15.7686	27.9696
124	O	19.7705	15.8536	18.6094
125	O	19.689	19.6015	28.1068
126	O	19.7711	20.0452	18.5744
127	O	19.6599	11.94	28.0332
128	O	19.7777	11.6616	18.4992
129	O	23.6587	15.8168	27.9532
130	O	23.5834	15.8685	18.6053
131	O	15.7791	15.7287	27.8367
132	O	15.9587	15.8391	18.5025
133	O	23.4788	19.6772	28.0767
134	O	23.4993	19.8697	18.6789
135	O	23.4691	11.9948	27.8804
136	O	23.49	11.8259	18.5624
137	O	15.8934	19.5177	27.851

138	O	16.0584	19.8912	18.5337
139	O	15.861	11.8968	27.8707
140	O	16.0481	11.8287	18.5068
141	O	21.6253	15.7413	29.6218
142	O	21.689	15.8327	20.265
143	O	13.8204	15.7366	29.4472
144	O	21.5784	19.8717	29.7804
145	O	21.6293	19.6318	20.3352
146	O	21.5912	11.6351	29.6699
147	O	21.6331	12.0965	20.2392
148	O	13.982	19.7923	29.4766
149	O	13.9451	11.8628	29.4635
150	O	25.5177	15.7632	29.6746
151	O	17.7259	15.7585	29.5724
152	O	17.8088	15.8485	20.2121
153	O	25.3669	19.6523	29.6878
154	O	25.3361	11.7039	29.5546
155	O	17.7164	19.8708	29.6966
156	O	17.8677	19.5822	20.2557
157	O	17.7207	11.633	29.641
158	O	17.8705	12.0404	20.2194
159	Ti	19.6617	15.7475	29.9731
160	Ti	19.7447	15.8362	20.5235
161	Ti	19.6674	19.4894	30.1622
162	Ti	19.7373	19.8641	20.5521
163	Ti	19.6307	12.0035	30.0877
164	Ti	19.7559	11.8058	20.4799
165	Ti	23.6663	15.7579	30.0317
166	Ti	23.4926	15.8184	20.447
167	Ti	15.6376	15.7372	29.9379
168	Ti	16.0006	15.8579	20.3479
169	Ti	23.5598	19.4372	30.215
170	Ti	23.4377	19.7135	20.5039
171	Ti	23.5323	12.0526	30.1177
172	Ti	23.4335	11.9301	20.4109

173	Ti	15.7705	19.4335	30.0869
174	Ti	16.0625	19.7536	20.383
175	Ti	15.7361	12.0634	30.0397
176	Ti	16.0571	11.9523	20.3362
177	O	19.6452	13.807	30.2583
178	O	19.7305	13.8846	20.8959
179	O	19.7214	21.6809	21.0403
180	O	19.6667	17.6809	30.2955
181	O	19.7483	17.781	20.9343
182	O	19.764	9.981	20.9365
183	O	23.4524	13.8603	30.2718
184	O	23.859	13.9027	20.8525
185	O	23.791	21.5018	21.1135
186	O	15.9131	13.864	30.198
187	O	15.623	13.8949	20.7611
188	O	15.8488	21.5426	20.9432
189	O	23.4027	17.6326	30.3383
190	O	23.8611	17.77	20.9156
191	O	23.6442	10.1297	20.9447
192	O	15.8699	17.6238	30.2056
193	O	15.622	17.7654	20.7697
194	O	15.698	10.1542	20.8995
195	O	19.6272	15.7278	31.9007
196	O	19.7119	15.8183	22.5434
197	O	19.6006	19.5342	32.0015
198	O	19.6748	19.7332	22.662
199	O	19.6186	11.9205	31.9274
200	O	19.7592	11.9009	22.5912
201	O	23.7927	15.7289	32.0315
202	O	23.5552	15.8054	22.4962
203	O	15.4267	15.7273	31.9192
204	O	15.8812	15.8342	22.394
205	O	23.6577	19.4476	32.0641
206	O	23.4443	19.6001	22.7367
207	O	23.637	12.0007	31.9467

208	O	23.578	12.0082	22.5781
209	O	15.5955	19.4471	31.9103
210	O	15.8423	19.6302	22.5309
211	O	15.5816	12.0167	31.8781
212	O	15.9612	12.0287	22.5676
213	Ti	19.6042	13.7674	32.3868
214	Ti	19.6896	13.9137	22.8222
215	Ti	19.7535	21.5418	22.8825
216	Ti	19.6012	17.6781	32.4228
217	Ti	19.7092	17.7153	22.8598
218	Ti	19.6788	10.0881	22.7792
219	Ti	23.3582	13.8146	32.4978
220	Ti	23.651	13.9067	22.8692
221	Ti	23.5943	21.3946	22.9261
222	Ti	15.861	13.8112	32.433
223	Ti	15.7769	13.9726	22.7582
224	Ti	15.9392	21.4903	22.7981
225	Ti	23.3531	17.6384	32.5551
226	Ti	23.6264	17.6549	22.9098
227	Ti	23.4999	10.1456	22.793
228	Ti	15.8563	17.6295	32.4501
229	Ti	15.7553	17.7285	22.7885
230	Ti	15.8302	10.2254	22.7222
231	O	16.854	14.161	14.3845
232	O	16.8435	17.6938	14.4072
233	O	22.788	14.0971	14.4395
234	O	22.7785	17.6109	14.4805
235	H	16.5725	15.0624	14.0994
236	H	16.3199	18.4367	14.0398
237	H	23.3224	13.3643	14.0675
238	H	23.0536	16.7114	14.1824
239	O	17.8446	18.6502	36.0845
240	O	21.42	12.6984	36.0729
241	O	17.8597	12.7404	36.0505
242	O	21.3781	18.6658	36.1394

243	H	18.737	18.9212	36.4044
244	H	22.1485	12.1264	36.3941
245	H	18.7498	12.4485	36.3573
246	H	22.1101	19.2054	36.5051
247	C	32.7454	16.196	28.3253
248	C	32.4336	16.2293	26.9558
249	C	31.1021	16.1286	26.533
250	C	30.0763	15.9932	27.4923
251	C	30.3899	15.9594	28.8672
252	C	31.726	16.0576	29.2941
253	C	32.0611	16.0185	30.7497
254	C	32.2634	14.805	31.4092
255	C	32.1619	13.5244	30.7529
256	C	32.3706	12.3603	31.4419
257	C	32.7166	12.3128	32.8964
258	C	32.8135	13.6454	33.5274
259	C	32.5977	14.8122	32.8242
260	O	32.709	16.0046	33.4887
261	C	32.5092	17.1903	32.8701
262	C	32.6402	18.3553	33.6494
263	C	32.4402	19.6269	33.0614
264	O	32.5697	20.7213	33.8218
265	C	32.1066	19.6819	31.6768
266	C	31.978	18.5346	30.9038
267	C	32.1791	17.2566	31.4846
268	Br	31.8352	21.4103	30.9163
269	Br	33.0784	18.2374	35.4761
270	Br	33.2484	13.6826	35.3572
271	O	32.9023	11.259	33.5016
272	Br	32.2322	10.6895	30.5818
273	C	28.6546	15.8847	27.0814
274	O	28.4177	15.9418	25.7923
275	O	27.7477	15.7473	27.9366
276	H	33.7955	16.2708	28.6525
277	H	33.2413	16.3318	26.2133

278	H	30.8451	16.1521	25.4632
279	H	31.9101	13.5003	29.6826
280	H	31.7164	18.6129	29.8389
281	H	27.3758	15.8615	25.6476
282	H	32.3897	21.5133	33.2494
283	H	29.5731	15.852	29.5984

Table S3. Cartesian coordinates of the optimized geometry of para-Eosin Y and anatase cluster

All coordinates are in angstroms.

1	O	21.6299	13.8758	23.2851
2	O	21.5361	13.883	32.6768
3	O	21.6718	21.7676	23.2833
4	O	13.9192	13.9106	23.3016
5	O	14.3203	22.1143	23.4898
6	O	21.6365	17.7208	23.2961
7	O	21.5487	17.518	32.7301
8	O	21.5994	9.6639	23.2423
9	O	13.9392	17.6611	23.2859
10	O	13.9879	10.0872	23.3938
11	O	25.4457	13.9449	23.4026
12	O	25.4226	21.456	23.6435
13	O	17.7566	13.8843	23.1966
14	O	17.6874	13.9126	32.6654
15	O	17.811	21.9488	23.3227
16	O	25.4536	17.7243	23.5183
17	O	25.1066	9.5136	23.4734
18	O	17.763	17.7386	23.2715
19	O	17.6988	17.518	32.684
20	O	17.7352	9.8396	23.1223
21	O	19.6408	13.94	24.8361
22	O	19.7748	13.9384	15.0152
23	O	19.6091	13.8847	34.2829
24	O	19.7573	21.9125	24.9351
25	O	19.7038	17.6279	24.8782
26	O	19.8119	17.8399	15.055
27	O	19.6122	17.49	34.3173
28	O	19.6178	9.6581	24.809
29	O	23.4862	13.8555	25.0005
30	O	23.4288	13.7757	34.2945
31	O	23.4146	21.9274	25.1492
32	O	15.8919	14.2851	24.8314

33	O	15.7583	13.8393	34.2353
34	O	16.0435	21.0105	24.9554
35	O	23.4446	17.2232	24.9574
36	O	23.4322	17.5476	34.3601
37	O	23.3342	10.524	24.9509
38	O	15.8541	17.752	24.942
39	O	15.7637	17.5942	34.249
40	O	15.9555	9.6592	24.9601
41	Ti	21.5124	13.9256	25.2574
42	Ti	21.4619	13.9214	15.7152
43	Ti	21.5613	13.9753	34.778
44	Ti	21.5672	21.4248	25.4088
45	Ti	14.1249	14.0398	25.112
46	Ti	14.2531	21.2209	25.1755
47	Ti	21.5192	17.6482	25.3027
48	Ti	21.509	17.8652	15.7493
49	Ti	21.5669	17.3666	34.8222
50	Ti	21.4233	10.2291	25.2763
51	Ti	14.0358	17.6745	25.1285
52	Ti	14.2454	10.3464	25.2084
53	Ti	25.2843	13.9	25.239
54	Ti	25.1046	21.1991	25.4358
55	Ti	17.7998	13.9165	25.2189
56	Ti	18.0611	13.898	15.6697
57	Ti	17.6128	13.9977	34.7668
58	Ti	17.9356	21.3309	25.3441
59	Ti	25.1751	17.5287	25.3121
60	Ti	25.1208	10.3456	25.1825
61	Ti	17.8012	17.647	25.2521
62	Ti	18.108	17.8432	15.7161
63	Ti	17.6195	17.4029	34.7885
64	Ti	17.7943	10.142	25.2545
65	O	21.4763	15.7511	25.6819
66	O	21.5868	15.8772	16.2243
67	O	21.5627	15.6601	35.4929

68	O	13.5514	15.8516	25.5615
69	O	21.6434	19.6069	25.5976
70	O	21.6978	19.7191	16.2914
71	O	21.1885	11.9912	25.591
72	O	21.6443	12.0571	16.185
73	O	13.5473	19.5168	25.4117
74	O	14.4333	12.1341	25.4442
75	O	25.9121	15.7133	25.6682
76	O	17.8419	15.8085	25.6173
77	O	17.973	15.8763	16.1809
78	O	17.6647	15.697	35.4465
79	O	24.8349	19.4163	25.6715
80	O	25.7856	12.0624	25.4722
81	O	18.1799	19.567	25.6294
82	O	17.9228	19.6978	16.219
83	O	17.7107	11.953	25.4706
84	O	17.8681	12.0328	16.1687
85	O	21.628	13.8215	27.2643
86	O	21.568	13.9374	17.8157
87	O	21.5321	21.5303	27.2447
88	O	13.5467	13.8719	27.133
89	O	13.9888	21.4849	26.98
90	O	21.6447	17.7046	27.2731
91	O	21.5768	17.7851	17.8566
92	O	21.5599	9.9855	27.0779
93	O	13.7298	17.7362	27.246
94	O	13.3781	10.3699	26.9015
95	O	25.6276	13.7937	27.3456
96	O	26.007	21.1297	27.1131
97	O	17.755	13.8245	27.1815
98	O	17.9478	13.9344	17.7751
99	O	17.7803	21.5428	27.1481
100	O	25.8072	17.6693	27.3012
101	O	25.4102	10.0447	26.9856
102	O	17.7723	17.7039	27.2545

103	O	17.9559	17.7831	17.8114
104	O	17.8267	10.0043	27.0905
105	Ti	21.6928	15.7401	27.6894
106	Ti	21.7239	15.8591	18.1282
107	Ti	13.9754	15.8298	27.613
108	Ti	21.6116	19.7057	27.7492
109	Ti	21.6976	19.6046	18.0932
110	Ti	21.493	11.8195	27.6602
111	Ti	21.6584	12.1109	18.0023
112	Ti	14.1177	19.6752	27.6663
113	Ti	13.9804	12.0111	27.617
114	Ti	25.5958	15.6696	27.8411
115	Ti	17.8344	15.7794	27.6434
116	Ti	17.7925	15.8555	18.0814
117	Ti	25.3639	19.5053	27.8212
118	Ti	25.2426	11.8251	27.714
119	Ti	17.8608	19.7009	27.6993
120	Ti	17.8643	19.6061	18.0342
121	Ti	17.7401	11.8161	27.6259
122	Ti	17.8261	12.1095	17.9717
123	O	19.7043	15.756	27.9618
124	O	19.7542	15.8521	18.602
125	O	19.7125	19.588	28.1007
126	O	19.7773	20.043	18.5719
127	O	19.6362	11.9283	28.0225
128	O	19.7365	11.6603	18.4862
129	O	23.6561	15.7802	27.9399
130	O	23.567	15.8465	18.5915
131	O	15.7778	15.7397	27.8355
132	O	15.9422	15.8587	18.5012
133	O	23.5038	19.6402	28.0626
134	O	23.5061	19.845	18.6704
135	O	23.444	11.958	27.8637
136	O	23.4489	11.8014	18.5435
137	O	15.915	19.5284	27.8527

138	O	16.0643	19.9098	18.5367
139	O	15.8375	11.9074	27.8666
140	O	16.0078	11.8499	18.5
141	O	21.6251	15.7159	29.611
142	O	21.6753	15.8166	20.2544
143	O	13.8221	15.7571	29.4497
144	O	21.6069	19.8475	29.771
145	O	21.637	19.618	20.3292
146	O	21.568	11.6097	29.6556
147	O	21.597	12.0819	20.2242
148	O	14.0084	19.8127	29.4823
149	O	13.9246	11.8838	29.4628
150	O	25.5138	15.7126	29.662
151	O	17.7273	15.7577	29.568
152	O	17.7951	15.8557	20.2076
153	O	25.3934	19.6008	29.6729
154	O	25.3142	11.6574	29.532
155	O	17.7444	19.8686	29.6947
156	O	17.8745	19.587	20.2557
157	O	17.6984	11.6308	29.6335
158	O	17.8345	12.0471	20.2096
159	Ti	19.6625	15.7351	29.9654
160	Ti	19.7314	15.8311	20.5161
161	Ti	19.6939	19.4765	30.156
162	Ti	19.7458	19.8588	20.549
163	Ti	19.6108	11.9908	30.0773
164	Ti	19.7187	11.801	20.4674
165	Ti	23.6644	15.7212	30.0192
166	Ti	23.4789	15.7911	20.4331
167	Ti	15.6399	15.7478	29.9374
168	Ti	15.9871	15.8751	20.3465
169	Ti	23.5861	19.4009	30.2025
170	Ti	23.4463	19.6866	20.495
171	Ti	23.5122	12.0161	30.0994
172	Ti	23.3965	11.9036	20.392

173	Ti	15.796	19.4433	30.0881
174	Ti	16.0705	19.7695	20.3855
175	Ti	15.7175	12.0737	30.0364
176	Ti	16.0208	11.9702	20.3295
177	O	19.6361	13.7941	30.2494
178	O	19.7062	13.8795	20.8864
179	O	19.7404	21.6751	21.0386
180	O	19.682	17.668	30.289
181	O	19.7479	17.7754	20.9295
182	O	19.7168	9.9757	20.922
183	O	23.4414	13.8232	30.2573
184	O	23.8355	13.8727	20.8351
185	O	23.8123	21.4718	21.105
186	O	15.906	13.873	30.1956
187	O	15.599	13.9144	20.7586
188	O	15.8683	21.5591	20.948
189	O	23.4148	17.5972	30.3264
190	O	23.8598	17.74	20.9038
191	O	23.5954	10.1009	20.9233
192	O	15.8836	17.6329	30.2059
193	O	15.6189	17.784	20.7715
194	O	15.6514	10.174	20.8919
195	O	19.6349	15.7144	31.8933
196	O	19.7061	15.811	22.5365
197	O	19.6309	19.521	31.9956
198	O	19.6906	19.726	22.6591
199	O	19.6041	11.9069	31.9172
200	O	19.7268	11.8933	22.579
201	O	23.7979	15.6891	32.0182
202	O	23.5472	15.7748	22.4817
203	O	15.4343	15.7378	31.9191
204	O	15.8746	15.8497	22.3933
205	O	23.6884	19.4096	32.0512
206	O	23.4612	19.5702	22.7284
207	O	23.6234	11.9606	31.9286

208	O	23.549	11.9779	22.5598
209	O	15.6257	19.4573	31.9119
210	O	15.8574	19.6455	22.535
211	O	15.5666	12.0272	31.8754
212	O	15.9315	12.0442	22.5621
213	Ti	19.601	13.7538	32.3773
214	Ti	19.6718	13.9064	22.8131
215	Ti	19.7791	21.5341	22.8806
216	Ti	19.621	17.665	32.4163
217	Ti	19.7144	17.7078	22.8549
218	Ti	19.6354	10.0811	22.765
219	Ti	23.3547	13.7762	32.4815
220	Ti	23.6351	13.8759	22.8528
221	Ti	23.6208	21.3638	22.9183
222	Ti	15.8585	13.8193	32.4312
223	Ti	15.759	13.9885	22.7558
224	Ti	15.9635	21.5049	22.8024
225	Ti	23.3729	17.6025	32.5418
226	Ti	23.6331	17.6233	22.8978
227	Ti	23.4571	10.1157	22.7717
228	Ti	15.8758	17.6378	32.4497
229	Ti	15.7591	17.7441	22.7899
230	Ti	15.7879	10.2416	22.7144
231	O	16.8265	14.183	14.3746
232	O	16.8357	17.7119	14.4007
233	O	22.7597	14.0841	14.4285
234	O	22.7691	17.6035	14.4741
235	H	16.5538	15.0867	14.0882
236	H	16.3231	18.4582	14.0249
237	H	23.2911	13.3489	14.0567
238	H	23.0426	16.7044	14.174
239	O	17.8743	18.6477	36.0803
240	O	21.4176	12.6756	36.0617
241	O	17.8608	12.7372	36.045
242	O	21.4138	18.6432	36.1296

243	H	18.7677	18.9158	36.3997
244	H	22.1436	12.0969	36.3764
245	H	18.751	12.4424	36.3485
246	H	22.1471	19.1882	36.4848
247	C	32.7278	16.2182	28.5078
248	C	32.4369	16.3027	27.1261
249	C	31.1222	16.1665	26.6645
250	C	30.0702	15.9582	27.5823
251	C	30.3522	15.8756	28.9625
252	C	31.6682	15.9994	29.4187
253	C	34.1224	16.3738	29.0112
254	C	34.8194	15.291	29.5558
255	C	34.2838	13.9525	29.6151
256	C	35.0059	12.9255	30.1608
257	C	36.3761	13.0929	30.7348
258	C	36.8954	14.4715	30.6325
259	C	36.1623	15.4972	30.0727
260	O	36.729	16.7415	30.0141
261	C	36.0769	17.8005	29.4851
262	C	36.7533	19.0354	29.4868
263	C	36.1239	20.1888	28.9634
264	O	36.7863	21.3524	28.9756
265	C	34.8015	20.0549	28.4506
266	C	34.1293	18.8389	28.4509
267	C	34.7567	17.6739	28.962
268	Br	33.9731	21.63	27.7631
269	Br	38.4947	19.169	30.1884
270	Br	38.6235	14.775	31.3105
271	O	37.0056	12.1643	31.2378
272	Br	34.3041	11.1784	30.2257
273	C	28.663	15.8356	27.1302
274	O	28.4534	15.9044	25.8359
275	O	27.7377	15.6788	27.9615
276	H	33.2561	16.4637	26.4068
277	H	30.9004	16.2233	25.5879

278	H	33.281	13.7655	29.2042
279	H	33.1043	18.78	28.0582
280	H	27.4179	15.8192	25.6685
281	H	36.1943	22.0453	28.5802
282	H	29.5226	15.7159	29.6691
283	H	31.8851	15.9385	30.4972

Table S4. Cartesian coordinates of the optimized geometry of orto-Eosin Y anchored by pyridine ring and anatase cluster. All coordinates are in angstroms.

1	O	29.811	14.8791	15.975
2	O	22.3529	12.8395	21.3377
3	O	28.7653	22.7024	17.6819
4	O	25.1252	15.5685	9.9103
5	O	24.1444	23.4488	11.9626
6	O	29.3029	18.6841	16.8036
7	O	21.8707	16.3585	22.0974
8	O	30.3684	10.8395	15.0999
9	O	24.6757	19.1988	10.6734
10	O	25.5811	11.8452	9.2575
11	O	32.0176	14.686	19.1001
12	O	30.6584	22.5319	20.5861
13	O	27.5284	15.2435	12.8952
14	O	20.0307	13.17	18.294
15	O	26.4398	23.0545	14.6014
16	O	31.5541	18.1048	19.8693
17	O	32.3107	10.3283	17.965
18	O	26.9832	19.0178	13.7199
19	O	19.5596	16.6786	19.0329
20	O	28.1042	11.3538	12.0082
21	O	27.3612	14.884	15.3718
22	O	35.1769	16.9661	9.7619
23	O	19.9278	12.6343	20.7425
24	O	26.3403	22.4679	17.0612
25	O	26.9444	18.1883	16.0972
26	O	34.6635	20.7421	10.5915
27	O	19.4492	16.1419	21.4879
28	O	27.9454	10.6115	14.4297
29	O	29.6161	14.2489	18.4196
30	O	22.2356	12.206	23.744
31	O	28.6481	21.2532	19.8452
32	O	25.0726	15.409	12.4227

33	O	17.6423	12.9045	17.66
34	O	24.2109	21.9118	13.9548
35	O	29.1	18.0834	19.257
36	O	21.7331	15.8908	24.5387
37	O	29.9606	11.1867	17.6263
38	O	24.5233	18.7755	13.1638
39	O	17.148	16.5625	18.4296
40	O	25.6125	10.9043	11.63
41	Ti	28.202	14.4996	17.0482
42	Ti	35.6532	16.6466	11.498
43	Ti	20.7029	12.4654	22.5917
44	Ti	27.1826	21.6398	18.6226
45	Ti	23.812	15.2663	11.141
46	Ti	22.9135	22.2034	12.7163
47	Ti	27.7062	18.084	17.8255
48	Ti	35.164	20.4502	12.3359
49	Ti	20.2576	15.759	23.2997
50	Ti	28.5948	10.9381	16.2436
51	Ti	23.2901	18.7945	11.8158
52	Ti	24.2874	11.6532	10.5609
53	Ti	30.4975	14.1734	20.0045
54	Ti	29.5447	21.224	21.4665
55	Ti	25.9744	14.8311	14.0977
56	Ti	33.6334	16.9335	8.7751
57	Ti	18.3254	12.8002	19.4658
58	Ti	25.0056	21.9687	15.7494
59	Ti	29.9953	17.7288	20.7948
60	Ti	30.8814	10.7719	19.1334
61	Ti	25.4849	18.4277	14.8723
62	Ti	33.1122	20.7447	9.6337
63	Ti	17.8761	16.1097	20.1692
64	Ti	26.4322	11.1534	13.3542
65	O	27.7542	16.1834	17.7982
66	O	35.0787	18.4118	12.2785
67	O	19.947	13.9553	23.345

68	O	22.8802	16.9719	11.3149
69	O	26.9787	19.8924	18.1851
70	O	34.6307	22.1117	13.1763
71	O	27.9416	12.595	16.5498
72	O	35.6402	14.7163	11.5476
73	O	22.5243	20.5577	11.9501
74	O	23.9757	13.316	11.2152
75	O	30.1658	15.8087	21.0163
76	O	25.3702	16.5651	14.683
77	O	32.9133	18.7463	9.3916
78	O	17.6135	14.3018	20.2406
79	O	29.8741	19.4167	21.751
80	O	30.8983	12.2992	20.1838
81	O	25.1545	20.1652	15.7754
82	O	32.3639	22.4487	10.1584
83	O	25.992	12.8707	13.8048
84	O	33.3603	15.0273	8.531
85	O	26.6532	13.96	18.2069
86	O	34.0531	16.1852	12.7804
87	O	25.8041	21.4323	19.8006
88	O	21.8788	14.7018	11.7965
89	O	21.2871	22.0801	13.5825
90	O	26.1318	17.692	19.0063
91	O	33.5575	19.9053	13.5853
92	O	27.3042	10.2869	17.3591
93	O	21.3927	18.412	12.7745
94	O	22.4237	11.3712	10.8357
95	O	29.0855	13.5613	21.483
96	O	28.1456	21.063	22.6734
97	O	24.3871	14.2939	15.15
98	O	31.9117	16.5027	9.9158
99	O	23.4381	21.796	16.6616
100	O	28.5373	17.3253	22.2535
101	O	29.6545	10.0604	20.3299
102	O	23.8555	18.0496	16.0065

103	O	31.3814	20.229	10.7189
104	O	25.0091	10.6078	14.3865
105	Ti	26.0984	15.7133	18.9115
106	Ti	33.6637	17.9629	13.4911
107	Ti	21.4991	16.4604	12.8
108	Ti	25.515	19.5398	19.63
109	Ti	33.2236	21.6091	14.1948
110	Ti	26.5412	11.9388	17.9834
111	Ti	34.208	14.3638	12.6117
112	Ti	21.0459	20.1647	13.7112
113	Ti	22.0074	12.7523	12.054
114	Ti	28.3984	15.3343	22.003
115	Ti	23.8036	16.0811	15.8519
116	Ti	31.3226	18.3102	10.3535
117	Ti	27.761	19.1422	22.5662
118	Ti	28.7605	11.6351	20.9851
119	Ti	23.2832	19.8751	16.6798
120	Ti	30.9215	21.9555	11.1445
121	Ti	24.3017	12.2531	14.9949
122	Ti	31.9145	14.6982	9.5607
123	O	24.7101	15.816	17.5078
124	O	32.0965	18.0267	12.1947
125	O	24.0712	19.5966	18.4008
126	O	31.6034	22.1043	13.0552
127	O	25.1077	12.0899	16.7498
128	O	32.7172	13.9786	11.2784
129	O	27.0737	15.455	20.6151
130	O	34.407	17.6835	15.2035
131	O	22.4226	16.1778	14.3425
132	O	29.8694	18.3689	9.1287
133	O	26.531	19.1223	21.2388
134	O	33.8397	21.5671	15.9845
135	O	27.5248	11.9034	19.6825
136	O	34.9011	13.8102	14.2829
137	O	22.009	19.8226	15.2137

138	O	29.3961	22.2773	10.0638
139	O	22.9404	12.4366	13.6547
140	O	30.4285	14.4857	8.376
141	O	24.5582	15.2854	19.9844
142	O	31.963	17.4944	14.6603
143	O	19.9721	15.9969	13.7307
144	O	23.952	19.2586	20.9039
145	O	31.4182	21.1015	15.4327
146	O	25.0398	11.2852	19.1575
147	O	32.4219	13.8627	13.8445
148	O	19.5379	19.9168	14.7128
149	O	20.5375	12.2232	13.0517
150	O	26.9188	14.9701	23.0935
151	O	22.2392	15.6609	16.8892
152	O	29.6502	17.8402	11.5807
153	O	26.376	18.8634	23.7389
154	O	27.3925	11.051	22.0528
155	O	21.6216	19.6062	17.7955
156	O	29.1749	21.4742	12.4431
157	O	22.7104	11.6285	16.0881
158	O	30.1643	14.1403	10.847
159	Ti	23.1146	15.3832	18.6529
160	Ti	30.5851	17.5992	13.2876
161	Ti	22.4863	18.9788	19.5323
162	Ti	30.0678	21.491	14.143
163	Ti	23.473	11.726	17.9226
164	Ti	31.1323	13.694	12.4418
165	Ti	25.5294	15.0166	21.8648
166	Ti	32.9038	17.2729	16.2043
167	Ti	20.6868	15.7326	15.4505
168	Ti	28.4486	17.974	10.2329
169	Ti	24.8578	18.5661	22.5864
170	Ti	32.3746	21.0391	16.9823
171	Ti	25.8089	11.4254	21.031
172	Ti	33.4019	13.5049	15.3334

173	Ti	20.1852	19.2719	16.4028
174	Ti	27.9689	21.7382	11.1108
175	Ti	21.1433	12.137	14.8396
176	Ti	28.9835	14.1918	9.4648
177	O	23.1087	13.4373	18.3965
178	O	30.5242	15.6156	13.0897
179	O	29.4481	23.1514	14.8029
180	O	22.6226	17.202	19.2302
181	O	30.0029	19.3938	13.9249
182	O	31.0105	11.8161	12.3346
183	O	25.3959	13.1469	21.436
184	O	33.0662	15.2856	16.341
185	O	31.8567	22.6402	17.8285
186	O	20.8888	13.8334	15.441
187	O	28.1324	16.0113	9.7695
188	O	27.1594	23.3743	11.6153
189	O	24.8823	16.798	22.1915
190	O	32.5725	18.9807	17.1574
191	O	33.3396	11.6184	15.4196
192	O	20.374	17.4805	16.1777
193	O	27.6483	19.7609	10.5806
194	O	28.5417	12.353	9.1337
195	O	21.584	14.9448	19.7404
196	O	28.9979	17.1286	14.4323
197	O	21.0163	18.6196	20.5688
198	O	28.3801	20.9124	15.3247
199	O	22.0388	11.236	18.9791
200	O	29.4582	13.3059	13.6798
201	O	24.0154	14.5431	23.1276
202	O	31.2729	16.7885	17.3825
203	O	19.0107	15.2952	16.4414
204	O	26.7854	17.496	11.3481
205	O	23.5065	18.1649	23.7704
206	O	30.835	20.4337	18.3611
207	O	24.4455	10.9552	22.1717

208	O	31.8051	13.0818	16.7169
209	O	18.6519	18.8937	17.3304
210	O	26.1585	21.1597	12.1343
211	O	19.6152	11.691	15.7805
212	O	27.1708	13.7651	10.7125
213	Ti	21.4402	12.9225	19.6042
214	Ti	28.999	15.2199	14.1902
215	Ti	28.0018	22.6266	15.814
216	Ti	20.9204	16.7139	20.4195
217	Ti	28.5002	18.8973	15.0203
218	Ti	29.5038	11.513	13.3525
219	Ti	23.6215	12.6198	22.6397
220	Ti	31.3702	14.8689	17.3322
221	Ti	30.3257	22.1973	18.7896
222	Ti	19.1223	13.2802	16.6897
223	Ti	26.6568	15.619	11.0749
224	Ti	25.768	22.8906	12.7397
225	Ti	23.1206	16.3178	23.4401
226	Ti	30.8824	18.5156	18.1574
227	Ti	31.8029	11.2391	16.3858
228	Ti	18.6206	16.9862	17.4766
229	Ti	26.1542	19.254	11.8527
230	Ti	27.1937	11.9958	10.3171
231	O	33.88	17.6177	7.1147
232	O	33.3958	21.024	7.8413
233	O	37.429	16.994	11.822
234	O	36.9661	20.3433	12.5129
235	H	33.8048	18.5823	6.923
236	H	33.3106	21.8825	7.3758
237	H	38.1324	16.316	11.9043
238	H	37.4525	19.4926	12.3911
239	O	16.8646	17.0051	21.3806
240	O	19.7444	10.9486	22.9743
241	O	17.6379	11.2707	20.1574
242	O	18.9666	16.7145	24.188

243	H	17.1454	17.1253	22.3181
244	H	19.9911	10.2704	23.6375
245	H	17.9836	10.863	20.9861
246	H	19.0574	17.1217	25.0749
247	C	33.2712	16.7377	27.2923
248	C	32.0988	15.9309	27.3795
249	C	31.7253	15.3979	28.633
250	C	32.4945	15.6312	29.781
251	C	33.652	16.4195	29.6943
252	C	34.0302	16.9689	28.4606
253	C	33.6943	17.3981	26.0209
254	C	34.8667	17.0192	25.3608
255	C	35.707	15.9344	25.809
256	C	36.8322	15.5782	25.1151
257	C	37.2789	16.261	23.8604
258	C	36.3807	17.3504	23.425
259	C	35.2513	17.7003	24.1343
260	O	34.4698	18.7139	23.6468
261	C	33.3284	19.0914	24.261
262	C	32.5894	20.1286	23.6535
263	C	31.3714	20.5444	24.2276
264	O	30.6382	21.5176	23.6172
265	C	30.9423	19.9373	25.4366
266	C	31.6894	18.938	26.0529
267	C	32.8914	18.4722	25.4659
268	Br	29.2787	20.4976	26.1779
269	Br	33.2026	20.9368	22.0738
270	Br	36.8434	18.2397	21.8355
271	O	38.2931	15.9312	23.2508
272	Br	37.9212	14.1597	25.7011
273	H	30.8273	14.7615	28.6949
274	H	35.4254	15.3909	26.723
275	H	31.342	18.5032	27.0
276	H	29.7736	21.6179	24.1134
277	H	34.2637	16.6138	30.5901

278	H	34.9269	17.6061	28.394
279	C	31.2553	15.6451	26.1881
280	C	31.8023	15.1587	24.9802
281	C	30.9681	14.97	23.8752
282	N	29.6477	15.2382	23.9065
283	C	29.0975	15.6516	25.0661
284	C	29.8593	15.859	26.2202
285	H	32.8735	14.9212	24.8958
286	H	31.3663	14.6081	22.9143
287	H	28.01	15.8355	25.0422
288	H	29.3676	16.2299	27.1335
289	H	32.1901	15.191	30.7443

Table S5. Cartesian coordinates of the optimized geometry of meta-Eosin Y anchored by

pyridine ring and anatase cluster. All coordinates are in angstroms.

1	O	22.8825	13.9468	20.5226
2	O	21.0475	13.9845	29.7419
3	O	24.0166	21.7478	20.7197
4	O	15.3849	15.054	19.137
5	O	16.8695	23.1289	19.5798
6	O	23.4158	17.754	20.6231
7	O	21.563	17.5709	29.8849
8	O	22.2835	9.7856	20.3706
9	O	15.9267	18.7695	19.2048
10	O	14.9101	11.2824	19.1497
11	O	26.5873	13.4841	21.3408
12	O	27.5534	20.9277	21.7569
13	O	19.1343	14.4976	19.729
14	O	17.3126	14.562	29.0302
15	O	20.2761	22.4788	20.0505
16	O	27.0991	17.2028	21.5467
17	O	25.6307	9.1472	21.2408
18	O	19.6559	18.317	19.8955
19	O	17.8274	18.1317	29.1392
20	O	18.5685	10.5007	19.5543
21	O	20.6758	14.3074	21.6878
22	O	22.6069	14.2509	12.0503
23	O	18.8765	14.2534	30.9701
24	O	21.8686	22.18	21.9936
25	O	21.2345	17.9391	21.8253
26	O	23.1861	18.1066	12.1895
27	O	19.3832	17.8243	31.0917
28	O	20.0644	10.0542	21.5495
29	O	24.3711	13.6585	22.5415
30	O	22.5728	13.5992	31.6738
31	O	25.3848	21.6767	22.8826
32	O	17.0796	15.177	21.0014

33	O	15.1338	14.7556	30.2119
34	O	18.1277	21.7974	21.3056
35	O	24.8049	17.0464	22.5745
36	O	23.0995	17.3346	31.8301
37	O	23.7719	10.4092	22.3831
38	O	17.493	18.5966	21.1873
39	O	15.6667	18.4823	30.3194
40	O	16.4766	10.5654	21.038
41	Ti	22.4188	14.0218	22.446
42	Ti	24.1156	14.0003	13.0489
43	Ti	20.6953	14.0642	31.8138
44	Ti	23.4718	21.4391	22.784
45	Ti	15.2729	15.1666	20.955
46	Ti	16.3726	22.2549	21.2022
47	Ti	22.9249	17.7075	22.5801
48	Ti	24.7116	17.8903	13.1866
49	Ti	21.1749	17.4194	31.9385
50	Ti	21.8121	10.3765	22.3533
51	Ti	15.6793	18.7744	21.0313
52	Ti	14.8673	11.4976	20.9857
53	Ti	26.091	13.4677	23.1113
54	Ti	26.8785	20.7223	23.4553
55	Ti	18.8114	14.5358	21.7267
56	Ti	20.8134	14.4582	12.3829
57	Ti	16.8606	14.6551	31.0809
58	Ti	19.9394	21.8558	22.0483
59	Ti	26.4719	17.0654	23.2551
60	Ti	25.4391	9.9697	22.941
61	Ti	19.318	18.2245	21.8464
62	Ti	21.4075	18.351	12.531
63	Ti	17.3447	18.0272	31.1852
64	Ti	18.278	10.7965	21.6723
65	O	22.5569	15.8347	22.8998
66	O	24.4125	15.9165	13.6227
67	O	20.812	15.7312	32.5585

68	O	14.8725	17.0408	21.3299
69	O	23.2548	19.6298	22.9415
70	O	25.0582	19.6991	13.7974
71	O	21.7587	12.1553	22.6644
72	O	23.9601	12.13	13.5016
73	O	15.4058	20.6682	21.262
74	O	15.2668	13.2377	21.3077
75	O	26.7541	15.182	23.718
76	O	19.0387	16.4032	22.1735
77	O	20.912	16.4279	12.9178
78	O	17.0257	16.332	31.7973
79	O	26.3435	18.9928	23.5913
80	O	26.274	11.5678	23.4056
81	O	19.8828	20.0753	22.3355
82	O	21.3953	20.2131	13.0342
83	O	18.4092	12.6027	21.9115
84	O	20.276	12.6403	12.7917
85	O	22.1428	13.9033	24.4342
86	O	23.8268	14.0061	15.1326
87	O	23.1155	21.5506	24.5858
88	O	14.3046	15.0855	22.8289
89	O	15.8184	22.5583	22.934
90	O	22.68	17.7481	24.5408
91	O	24.3731	17.8099	15.2662
92	O	21.5764	10.117	24.1416
93	O	14.998	18.8878	23.062
94	O	13.7	11.6483	22.4788
95	O	26.0039	13.2985	25.2608
96	O	27.437	20.5313	25.2705
97	O	18.3787	14.4546	23.641
98	O	20.3246	14.5127	14.4324
99	O	19.4846	22.0942	23.7972
100	O	26.7489	17.133	25.3322
101	O	25.3322	9.6187	24.7561
102	O	18.9272	18.2922	23.8148

103	O	20.8595	18.3213	14.561
104	O	17.9566	10.6626	23.4796
105	Ti	22.3705	15.8011	24.9135
106	Ti	24.1948	15.8844	15.5196
107	Ti	14.9029	16.9695	23.4255
108	Ti	22.8457	19.7348	25.0519
109	Ti	24.7031	19.5941	15.5645
110	Ti	21.6504	11.9455	24.7482
111	Ti	23.6409	12.1856	15.291
112	Ti	15.5688	20.7519	23.593
113	Ti	14.382	13.1868	23.3396
114	Ti	26.1316	15.1721	25.705
115	Ti	18.6403	16.3822	24.1633
116	Ti	20.3822	16.4377	14.7525
117	Ti	26.458	19.0102	25.8022
118	Ti	25.2855	11.4086	25.4817
119	Ti	19.2084	20.2584	24.3132
120	Ti	20.9862	20.1395	14.8049
121	Ti	18.0123	12.4724	24.0292
122	Ti	19.9164	12.7236	14.5594
123	O	20.3991	16.0856	24.8165
124	O	22.192	16.1567	15.6238
125	O	20.9182	19.8902	25.0508
126	O	22.8084	20.3057	15.6958
127	O	19.7977	12.3247	24.7744
128	O	21.6172	12.0091	15.4044
129	O	24.2383	15.5689	25.526
130	O	25.8997	15.6092	16.3109
131	O	16.6045	16.6258	23.9693
132	O	18.5048	16.6994	14.8233
133	O	24.6193	19.3957	25.7061
134	O	26.3871	19.5768	16.4713
135	O	23.5273	11.796	25.3163
136	O	25.2446	11.6428	16.1436
137	O	17.2639	20.3603	24.1049

138	O	19.1838	20.6928	14.9752
139	O	16.1279	12.8196	23.9309
140	O	18.0132	12.7226	14.7397
141	O	21.95	15.7818	26.7916
142	O	23.7514	15.8645	17.5982
143	O	14.4093	16.9289	25.1995
144	O	22.4892	19.8687	27.0442
145	O	24.2304	19.6189	17.7528
146	O	21.3273	11.72	26.722
147	O	23.1664	12.1652	17.4633
148	O	15.1446	20.9042	25.3613
149	O	13.9678	13.0726	25.1407
150	O	25.7409	15.2026	27.5296
151	O	18.1797	16.3726	26.0294
152	O	19.9908	16.4427	16.8406
153	O	26.1564	19.0912	27.633
154	O	25.012	11.2474	27.2845
155	O	18.7484	20.4448	26.2606
156	O	20.583	20.1263	16.9901
157	O	17.574	12.2913	25.994
158	O	19.503	12.6681	16.7568
159	Ti	19.9991	16.0727	26.7826
160	Ti	21.8134	16.1485	17.5006
161	Ti	20.5029	19.7745	27.063
162	Ti	22.3854	20.1318	17.6308
163	Ti	19.3983	12.3768	26.7907
164	Ti	21.2544	12.163	17.3524
165	Ti	23.9026	15.4866	27.5559
166	Ti	25.4701	15.5829	18.1042
167	Ti	16.0885	16.6588	26.0129
168	Ti	18.2086	16.7155	16.6454
169	Ti	24.2715	19.1404	27.8159
170	Ti	25.97	19.4341	18.2506
171	Ti	23.1956	11.8524	27.5201
172	Ti	24.8651	11.7495	17.9538

173	Ti	16.7222	20.2934	26.2771
174	Ti	18.8279	20.558	16.7911
175	Ti	15.6329	13.0099	26.0363
176	Ti	17.7047	12.8465	16.5431
177	O	19.6358	14.1592	27.0103
178	O	21.4552	14.2191	17.8139
179	O	22.5422	21.9319	18.157
180	O	20.2089	17.9883	27.1459
181	O	22.0234	18.0701	17.9551
182	O	20.9121	10.3566	17.7535
183	O	23.3366	13.6507	27.7057
184	O	25.4823	13.6358	18.52
185	O	26.461	21.15	18.9627
186	O	16.0288	14.7667	26.2722
187	O	17.4808	14.8287	16.9354
188	O	18.7733	22.3586	17.349
189	O	23.8308	17.38	27.8647
190	O	26.0335	17.4516	18.6833
191	O	24.7215	9.9367	18.4705
192	O	16.5408	18.4896	26.3695
193	O	18.0411	18.6572	17.0419
194	O	16.9917	11.1212	16.9893
195	O	19.5995	16.0632	28.6693
196	O	21.4118	16.1349	19.4793
197	O	20.1173	19.829	28.8628
198	O	21.9196	20.0119	19.689
199	O	19.0364	12.2978	28.5953
200	O	20.8887	12.2541	19.4336
201	O	23.6458	15.4387	29.5574
202	O	25.1472	15.5598	20.1312
203	O	15.5156	16.6836	27.9228
204	O	17.724	16.7088	18.635
205	O	24.0367	19.1363	29.6545
206	O	25.5601	19.3208	20.446
207	O	22.9645	11.7853	29.3396

208	O	24.6209	11.8048	20.1088
209	O	16.217	20.3355	28.0384
210	O	18.2018	20.4701	18.8593
211	O	15.1409	12.9877	27.816
212	O	17.2274	12.9347	18.7274
213	Ti	19.2026	14.1274	29.0897
214	Ti	21.0732	14.2536	19.7041
215	Ti	22.217	21.7886	19.9695
216	Ti	19.7661	17.995	29.2277
217	Ti	21.6337	18.0098	19.8423
218	Ti	20.516	10.4732	19.5533
219	Ti	22.8379	13.6223	29.8768
220	Ti	24.9122	13.6689	20.469
221	Ti	25.9243	21.0756	20.7075
222	Ti	15.5641	14.7231	28.4572
223	Ti	17.2896	14.8836	18.9339
224	Ti	18.5136	22.2958	19.1888
225	Ti	23.3844	17.3928	30.0313
226	Ti	25.4244	17.3735	20.606
227	Ti	24.2386	9.9744	20.2595
228	Ti	16.113	18.5027	28.5723
229	Ti	17.8031	18.6001	19.0541
230	Ti	16.8078	11.1723	18.808
231	O	19.8845	14.9196	10.8967
232	O	20.3915	18.392	11.0037
233	O	25.6376	13.9873	12.0223
234	O	26.1356	17.431	12.1646
235	H	19.801	15.8551	10.5946
236	H	20.1001	19.2006	10.5323
237	H	26.1376	13.1897	11.7484
238	H	26.3167	16.4944	11.9109
239	O	17.5355	19.2284	32.5304
240	O	20.1261	12.8042	33.0193
241	O	16.6928	13.3784	32.3571
242	O	20.9693	18.7043	33.2315

243	H	18.3892	19.3645	33.0045
244	H	20.6935	12.15	33.4786
245	H	17.469	12.9594	32.797
246	H	21.6988	19.1519	33.7092
247	C	34.5346	15.3822	28.1518
248	C	33.2238	15.4494	27.6375
249	C	32.3011	14.3984	27.8331
250	C	32.7166	13.2582	28.5582
251	C	34.0216	13.1751	29.0619
252	C	34.9281	14.2288	28.866
253	C	35.4721	16.5247	27.9563
254	C	36.6099	16.401	27.1529
255	C	36.9515	15.1926	26.4421
256	C	38.0807	15.1202	25.6716
257	C	39.0347	16.2574	25.495
258	C	38.6333	17.4823	26.2158
259	C	37.4926	17.5443	26.989
260	O	37.1928	18.7288	27.6067
261	C	36.0975	18.8724	28.3853
262	C	35.8905	20.1345	28.9747
263	C	34.7733	20.3497	29.8149
264	O	34.5944	21.5585	30.3615
265	C	33.8889	19.2569	30.045
266	C	34.0895	18.0107	29.4643
267	C	35.1962	17.7897	28.6047
268	Br	32.3999	19.571	31.1959
269	Br	37.0945	21.5457	28.6561
270	Br	39.7578	18.9782	26.0256
271	O	40.0489	16.1749	24.8049
272	Br	38.5186	13.5385	24.7456
273	H	32.9108	16.3548	27.0929
274	H	36.2827	14.3238	26.5247
275	H	33.3903	17.1897	29.676
276	H	33.7701	21.5251	30.9151
277	H	34.3391	12.2766	29.6152

278	H	35.9486	14.1661	29.2767
279	C	30.9201	14.5129	27.3046
280	C	30.6462	15.1399	26.0674
281	C	29.3253	15.2709	25.6331
282	N	28.2762	14.8263	26.3547
283	C	28.5172	14.2073	27.5294
284	C	29.8091	14.0254	28.0291
285	H	31.4611	15.5135	25.4282
286	H	29.0825	15.7511	24.672
287	H	27.6273	13.8801	28.0918
288	H	29.9408	13.5425	29.0098
289	H	32.0205	12.4165	28.7045

Table S6. Cartesian coordinates of the optimized geometry of para-Eosin Y anchored by pyridine ring and anatase cluster. All coordinates are in angstroms.

1	O	21.5073	13.7482	23.2158
2	O	21.5214	13.7162	32.6066
3	O	21.8995	21.6289	23.266
4	O	13.8088	14.1291	23.3234
5	O	14.5729	22.2966	23.5551
6	O	21.6846	17.5933	23.2503
7	O	21.6822	17.331	32.6938
8	O	21.2876	9.543	23.1478
9	O	13.9992	17.8682	23.3319
10	O	13.7079	10.3018	23.3912
11	O	25.3243	13.6539	23.2945
12	O	25.6338	21.1702	23.5803
13	O	17.6387	13.9307	23.1758
14	O	17.6763	13.8909	32.6472
15	O	18.0506	21.9836	23.3491
16	O	25.5116	17.4057	23.4294
17	O	24.7843	9.2347	23.3333
18	O	17.819	17.7825	23.2756
19	O	17.839	17.5031	32.6926
20	O	17.4349	9.8905	23.0766
21	O	19.5424	13.9027	24.7917
22	O	19.5686	13.9527	14.9686
23	O	19.6156	13.774	34.239
24	O	20.0098	21.8575	24.9382
25	O	19.7718	17.5648	24.8571
26	O	19.7849	17.8425	15.0327
27	O	19.7669	17.3843	34.3038
28	O	19.3284	9.6151	24.7393
29	O	23.3737	13.5995	24.9083
30	O	23.4255	13.4983	34.2016
31	O	23.6629	21.7037	25.1177
32	O	15.8129	14.4012	24.8343

33	O	15.7662	13.8995	34.24
34	O	16.264	21.1109	24.9945
35	O	23.4895	17.0435	24.8862
36	O	23.5841	17.2643	34.2996
37	O	23.0773	10.3242	24.8336
38	O	15.9328	17.8669	24.9675
39	O	15.9266	17.6524	34.2778
40	O	15.6719	9.786	24.9365
41	Ti	21.415	13.7922	25.1934
42	Ti	21.2611	13.8556	15.6486
43	Ti	21.5756	13.7796	34.7091
44	Ti	21.7998	21.2822	25.3915
45	Ti	14.0392	14.2371	25.1334
46	Ti	14.4879	21.3993	25.2379
47	Ti	21.5935	17.5114	25.2654
48	Ti	21.4894	17.7903	15.7084
49	Ti	21.7195	17.1667	34.7841
50	Ti	21.161	10.1056	25.1887
51	Ti	14.1157	17.8679	25.1722
52	Ti	13.9957	10.5406	25.2055
53	Ti	25.1777	13.594	25.1218
54	Ti	25.327	20.9075	25.3787
55	Ti	17.708	13.9542	25.203
56	Ti	17.8599	13.9831	15.6385
57	Ti	17.6318	13.9712	34.7486
58	Ti	18.1717	21.347	25.3665
59	Ti	25.2486	17.2238	25.2315
60	Ti	24.854	10.0516	25.0473
61	Ti	17.8791	17.6748	25.2507
62	Ti	18.0886	17.9179	15.7102
63	Ti	17.7777	17.3761	34.7962
64	Ti	17.535	10.1815	25.2109
65	O	21.481	15.6136	25.6288
66	O	21.4854	15.7978	16.1697
67	O	21.6545	15.4551	35.4404

68	O	13.5516	16.0669	25.6007
69	O	21.7881	19.4619	25.573
70	O	21.7669	19.6294	16.2605
71	O	20.998	11.8727	25.5171
72	O	21.3588	11.9815	16.1043
73	O	13.7104	19.7277	25.4719
74	O	14.2599	12.3169	25.4499
75	O	25.7637	15.375	25.61
76	O	17.833	15.8359	25.6106
77	O	17.8655	15.9577	16.1655
78	O	17.763	15.6627	35.437
79	O	24.9938	19.1388	25.5964
80	O	25.6131	11.7244	25.3549
81	O	18.3461	19.5728	25.6389
82	O	17.993	19.7745	16.2267
83	O	17.5401	11.9922	25.4405
84	O	17.5824	12.126	16.1288
85	O	21.5333	13.6679	27.197
86	O	21.3898	13.8514	17.7483
87	O	21.781	21.3781	27.2293
88	O	13.4718	14.0797	27.159
89	O	14.2536	21.6645	27.0475
90	O	21.7367	17.5469	27.2351
91	O	21.571	17.6925	17.8137
92	O	21.3164	9.8442	26.9864
93	O	13.825	17.9319	27.2967
94	O	13.1535	10.5883	26.9113
95	O	25.5858	13.4385	27.2452
96	O	26.2339	20.7923	27.0505
97	O	17.6768	13.8468	27.1631
98	O	17.7729	14.0088	17.7459
99	O	18.0391	21.5535	27.1734
100	O	25.8834	17.3443	27.2118
101	O	25.1373	9.7086	26.8458
102	O	17.8651	17.7222	27.2581

103	O	17.9518	17.8508	17.8071
104	O	17.5789	10.0282	27.0449
105	Ti	21.6828	15.5806	27.6412
106	Ti	21.6367	15.7603	18.0741
107	Ti	13.9897	16.0143	27.6506
108	Ti	21.7873	19.55	27.7223
109	Ti	21.7772	19.5022	18.0622
110	Ti	21.3272	11.6765	27.5815
111	Ti	21.3952	12.0215	17.9218
112	Ti	14.306	19.8478	27.7242
113	Ti	13.831	12.1992	27.628
114	Ti	25.57	15.3093	27.6752
115	Ti	17.8387	15.7979	27.6418
116	Ti	17.7063	15.9317	18.0697
117	Ti	25.5244	19.1833	27.7408
118	Ti	25.0721	11.4876	27.5882
119	Ti	18.0443	19.7065	27.7144
120	Ti	17.9472	19.6743	18.043
121	Ti	17.5778	11.8392	27.5929
122	Ti	17.5672	12.1913	17.9336
123	O	19.7134	15.6871	27.9305
124	O	19.672	15.8381	18.5678
125	O	19.894	19.5072	28.0978
126	O	19.8826	20.0242	18.5638
127	O	19.4813	11.8561	27.9701
128	O	19.461	11.6518	18.4252
129	O	23.648	15.5061	27.8727
130	O	23.4812	15.6632	18.5183
131	O	15.7892	15.8446	27.848
132	O	15.8626	16.0125	18.5101
133	O	23.6804	19.4062	28.0159
134	O	23.6003	19.6542	18.621
135	O	23.2896	11.735	27.7563
136	O	23.1762	11.6292	18.439
137	O	16.0964	19.618	27.8906

138	O	16.1683	20.0539	18.5666
139	O	15.6839	12.0122	27.8559
140	O	15.7452	12.0136	18.4834
141	O	21.6423	15.5392	29.5649
142	O	21.6063	15.7096	20.1993
143	O	13.8564	15.9313	29.4868
144	O	21.8163	19.6806	29.7473
145	O	21.7392	19.5062	20.2979
146	O	21.4213	11.4601	29.573
147	O	21.358	11.9817	20.1437
148	O	14.2238	19.9824	29.5429
149	O	13.7898	12.0651	29.4744
150	O	25.5518	15.4284	29.5391
151	O	17.7542	15.7685	29.5592
152	O	17.7317	15.9187	20.1945
153	O	25.5919	19.2259	29.5993
154	O	25.1556	11.3059	29.4058
155	O	17.9588	19.8699	29.7126
156	O	17.9792	19.6407	20.2644
157	O	17.5496	11.6398	29.6013
158	O	17.5993	12.1124	20.1713
159	Ti	19.7112	15.6539	29.9384
160	Ti	19.6675	15.8084	20.4825
161	Ti	19.8951	19.3896	30.1522
162	Ti	19.8623	19.8284	20.5409
163	Ti	19.4805	11.9153	30.0227
164	Ti	19.4723	11.7821	20.4088
165	Ti	23.735	15.468	29.9297
166	Ti	23.4084	15.6032	20.3614
167	Ti	15.6815	15.8424	29.9538
168	Ti	15.9279	16.0184	20.3555
169	Ti	23.78	19.129	30.148
170	Ti	23.5511	19.4902	20.4468
171	Ti	23.3845	11.7723	29.9965
172	Ti	23.1491	11.722	20.2893

173	Ti	15.9987	19.528	30.1276
174	Ti	16.1865	19.9016	20.4155
175	Ti	15.5951	12.1689	30.0289
176	Ti	15.7857	12.1178	20.3141
177	O	19.5768	13.7135	30.2062
178	O	19.5573	13.8552	20.8409
179	O	19.9399	21.6409	21.0419
180	O	19.8015	17.5828	30.2748
181	O	19.7765	17.7453	20.9076
182	O	19.3966	9.9547	20.8524
183	O	23.4227	13.5798	30.1694
184	O	23.6826	13.6659	20.7449
185	O	24.0007	21.2553	21.0606
186	O	15.8661	13.956	30.1982
187	O	15.4554	14.0749	20.7615
188	O	16.0709	21.6942	20.9911
189	O	23.4995	17.341	30.2628
190	O	23.8864	17.5248	20.8363
191	O	23.2681	9.9073	20.8044
192	O	15.9998	17.7147	30.2352
193	O	15.6496	17.9373	20.7971
194	O	15.3445	10.3357	20.8697
195	O	19.6828	15.6211	31.8654
196	O	19.6641	15.7736	22.5019
197	O	19.8498	19.4242	31.9933
198	O	19.824	19.6848	22.6504
199	O	19.5065	11.8163	31.8619
200	O	19.5076	11.8588	22.5211
201	O	23.8713	15.4144	31.9414
202	O	23.4939	15.5663	22.41
203	O	15.496	15.8265	31.9386
204	O	15.844	15.9832	22.4036
205	O	23.9157	19.1178	31.9961
206	O	23.5929	19.3592	22.6752
207	O	23.5021	11.6976	31.824

208	O	23.3362	11.7724	22.4511
209	O	15.8524	19.5376	31.9541
210	O	15.9921	19.7732	22.5667
211	O	15.4618	12.1159	31.8699
212	O	15.7276	12.1793	22.5484
213	Ti	19.5776	13.6596	32.3332
214	Ti	19.5421	13.872	22.7679
215	Ti	19.9938	21.4853	22.8821
216	Ti	19.7616	17.568	32.4015
217	Ti	19.7718	17.6656	22.8352
218	Ti	19.3394	10.0515	22.6967
219	Ti	23.3294	13.5236	32.3882
220	Ti	23.4945	13.6633	22.764
221	Ti	23.8264	21.1452	22.876
222	Ti	15.8422	13.8882	32.4338
223	Ti	15.6433	14.1278	22.758
224	Ti	16.1815	21.6229	22.8453
225	Ti	23.5061	17.328	32.4806
226	Ti	23.6825	17.4077	22.8381
227	Ti	23.1551	9.9166	22.6552
228	Ti	16.0218	17.7042	32.477
229	Ti	15.8178	17.8767	22.8168
230	Ti	15.5045	10.3844	22.6917
231	O	16.6302	14.3379	14.3546
232	O	16.8004	17.853	14.4035
233	O	22.5513	13.9621	14.3466
234	O	22.7259	17.4813	14.4189
235	H	16.3987	15.2584	14.0851
236	H	16.3235	18.6266	14.0358
237	H	23.029	13.1997	13.9575
238	H	22.9523	16.571	14.1133
239	O	18.0983	18.5978	36.0972
240	O	21.3903	12.4759	35.9844
241	O	17.8428	12.6959	36.0195
242	O	21.6435	18.4373	36.1062

243	H	19.0071	18.8233	36.4057
244	H	22.0914	11.8552	36.274
245	H	18.7252	12.3602	36.3033
246	H	22.4099	18.9342	36.4617
247	C	34.8764	16.5752	27.929
248	C	34.1752	16.4151	26.7124
249	C	32.8058	16.1262	26.7072
250	C	32.0815	16.0064	27.9164
251	C	32.7866	16.1656	29.1317
252	C	34.1599	16.4375	29.1391
253	C	36.3305	16.8965	27.9325
254	C	37.2749	15.9891	28.4242
255	C	36.9317	14.6809	28.9273
256	C	37.8934	13.8303	29.4026
257	C	39.3493	14.1675	29.4391
258	C	39.6605	15.5016	28.8877
259	C	38.6832	16.3495	28.4087
260	O	39.0695	17.5605	27.9001
261	C	38.1756	18.452	27.4175
262	C	38.6856	19.6691	26.9256
263	C	37.8049	20.656	26.4248
264	O	38.3123	21.8041	25.9584
265	C	36.4077	20.3795	26.4485
266	C	35.9013	19.1789	26.9311
267	C	36.7774	18.1741	27.4163
268	Br	35.2418	21.7389	25.79
269	Br	40.5385	19.9992	26.9323
270	Br	41.4739	16.0003	28.86
271	O	40.2006	13.3969	29.8784
272	Br	37.4364	12.1222	30.0543
273	H	34.7148	16.5137	25.7565
274	H	32.2845	16.0254	25.7416
275	H	35.877	14.3708	28.9172
276	H	34.8158	19.0083	26.9426
277	H	37.5553	22.3738	25.6592

278	H	32.2594	16.0521	30.0927
279	H	34.6882	16.5547	30.099
280	C	30.622	15.7483	27.9052
281	C	30.0086	14.9634	26.9008
282	C	28.6229	14.7888	26.9054
283	N	27.8242	15.3419	27.8394
284	C	28.3906	16.0716	28.8236
285	C	29.7673	16.2949	28.8903
286	H	30.6074	14.4705	26.1198
287	H	28.1197	14.1895	26.1299
288	H	27.6962	16.4959	29.5679
289	H	30.1652	16.9311	29.6959

Table S7. Total energies of the isolated Eosin Y / anatase and their complexes.

Species	Total energy (a.u.)
Anatase	-16526.8715
Orto-Eosin Y	-11436.4914
Meta-Eosin Y	-11436.4950
Para-Eosin Y	-11436.4885
Orto-Eosin Y + anatase	-27963.4327
Meta-Eosin Y + anatase	-27963.4115
Para-Eosin Y + anatase	-27963.4117
Orto-Eosin Y-pyridine	-11494.9020
Meta-Eosin Y-pyridine	-11494.9065
Para-Eosin Y-pyridine	-11494.9078
Orto-Eosin Y-pyridine + anatase	-28021.8359
Meta-Eosin Y-pyridine + anatase	-28021.8224
Para-Eosin Y-pyridine + anatase	-28021.8252

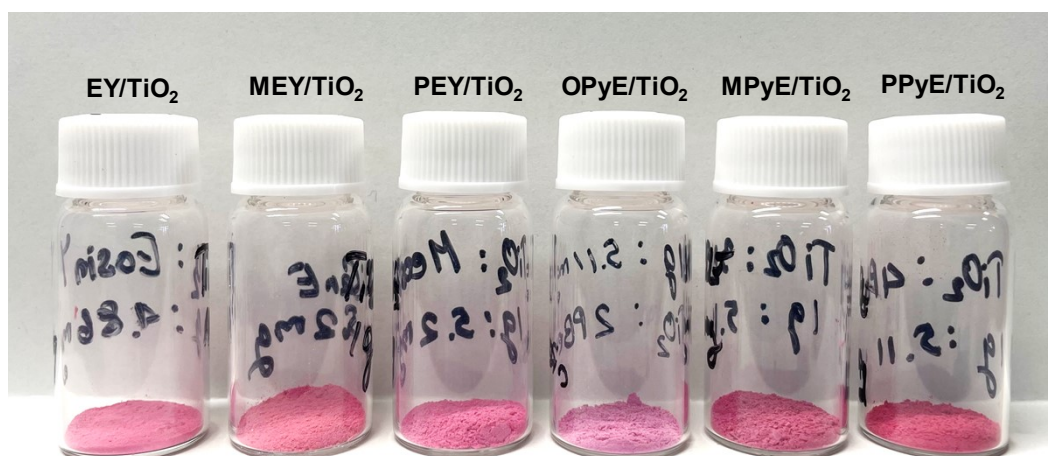


Figure S1. Dye/TiO₂ powder prepared as mentioned in the method and utilized in our studies.

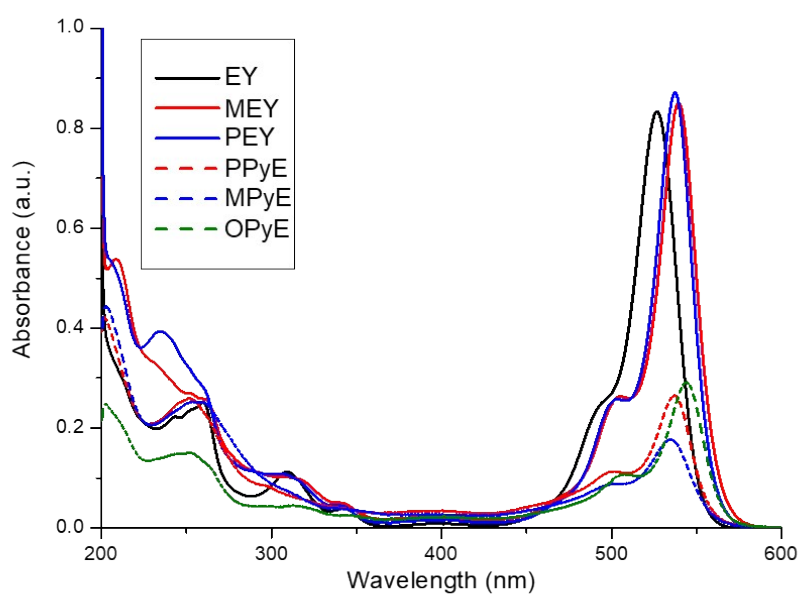


Figure S2. UV-Vis spectra of 1 M aqueous solution of modified EY

Table S8. The ratio of PL intensity/UV absorbance at 520 nm on all dye-modified TiO₂.

Dye/TiO ₂	PL intensity (a.u.)	UV/Vis absorbance at 520 nm (a.u.)	Normalized PL(a.u.)
EY/TiO ₂	17.72	0.805	22.01
MEY/TiO ₂	13.44	0.868	15.48
PEY/TiO ₂	10.93	0.566	19.31
OPyE/TiO ₂	4.58	0.200	22.90
MPyE/TiO ₂	6.36	0.220	28.89
PPyE/TiO ₂	5.49	0.295	18.61

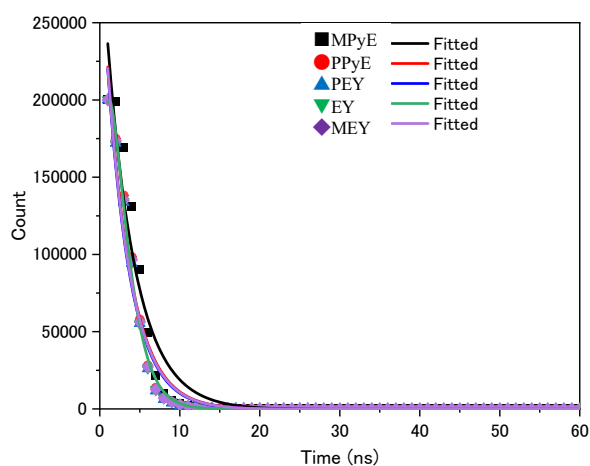


Figure S3. Transient PL spectra of EY modified TiO₂.

Table. S9 Flitting values of dye

	t ₁ (ns)
MPyE	3.59
PPyE	3.03
PEY	2.95
EY	2.97
MEY	2.99

$$\left| \frac{\Delta OD}{\Delta OD_0} \right| = A_0 + A_1 \exp \left[-\frac{t}{\tau_1} \right]$$

t : experimental data (ps)

τ_1, τ_2 : time decay constants (ps)

A_0, A_1, A_2 : constant values

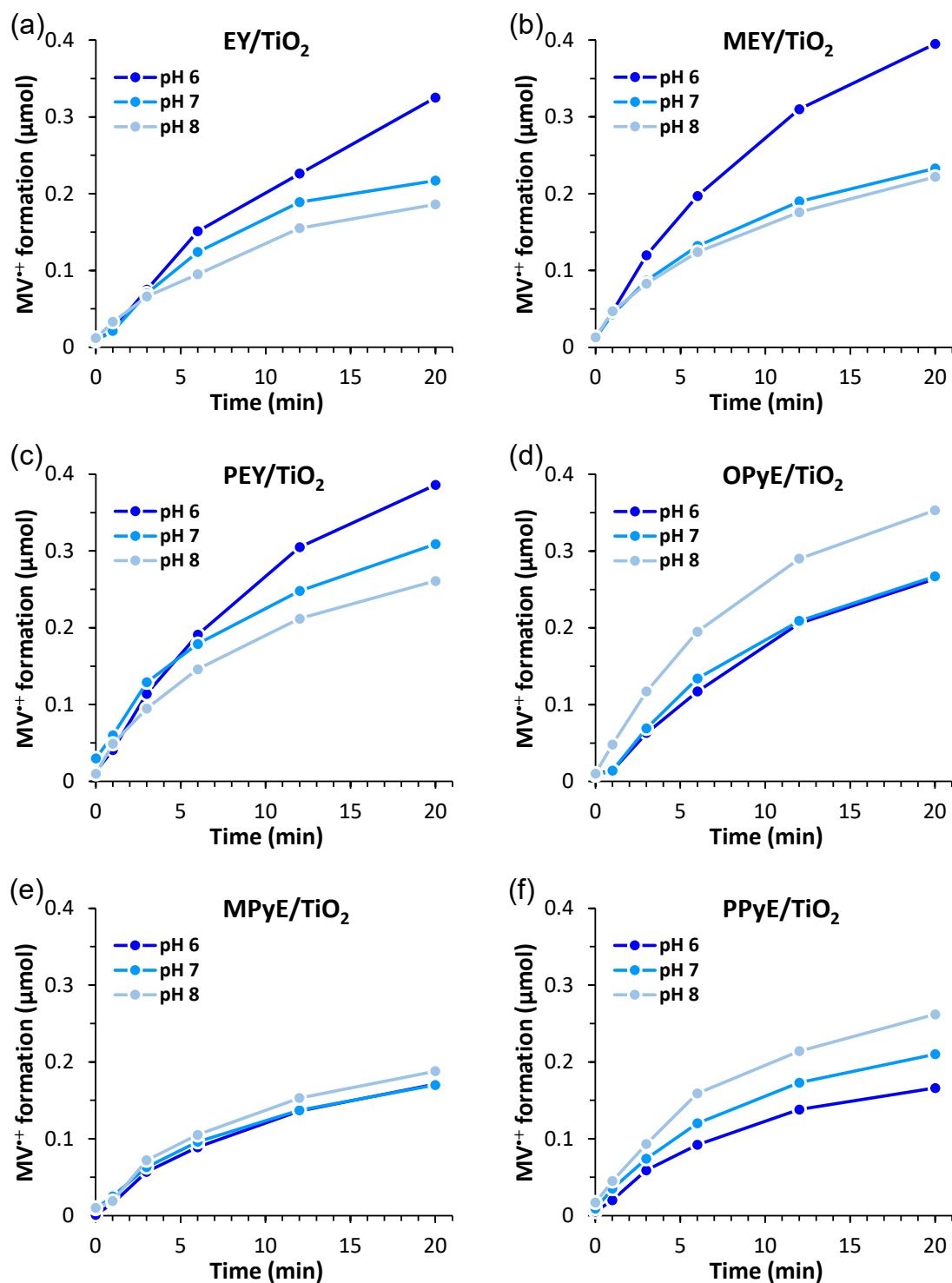


Figure S4. Effect of pH on photocatalytic methyl viologen (MV^{2+}) reduction by different dye/ TiO_2 nanoparticles. The reaction mixture consists of 100 mM L-cysteine pH 6-8, 1 mg/mL dye/ TiO_2 composite, 5 mM MV^{2+} solution in total volume of 3 mL under visible light illumination at 520 nm.

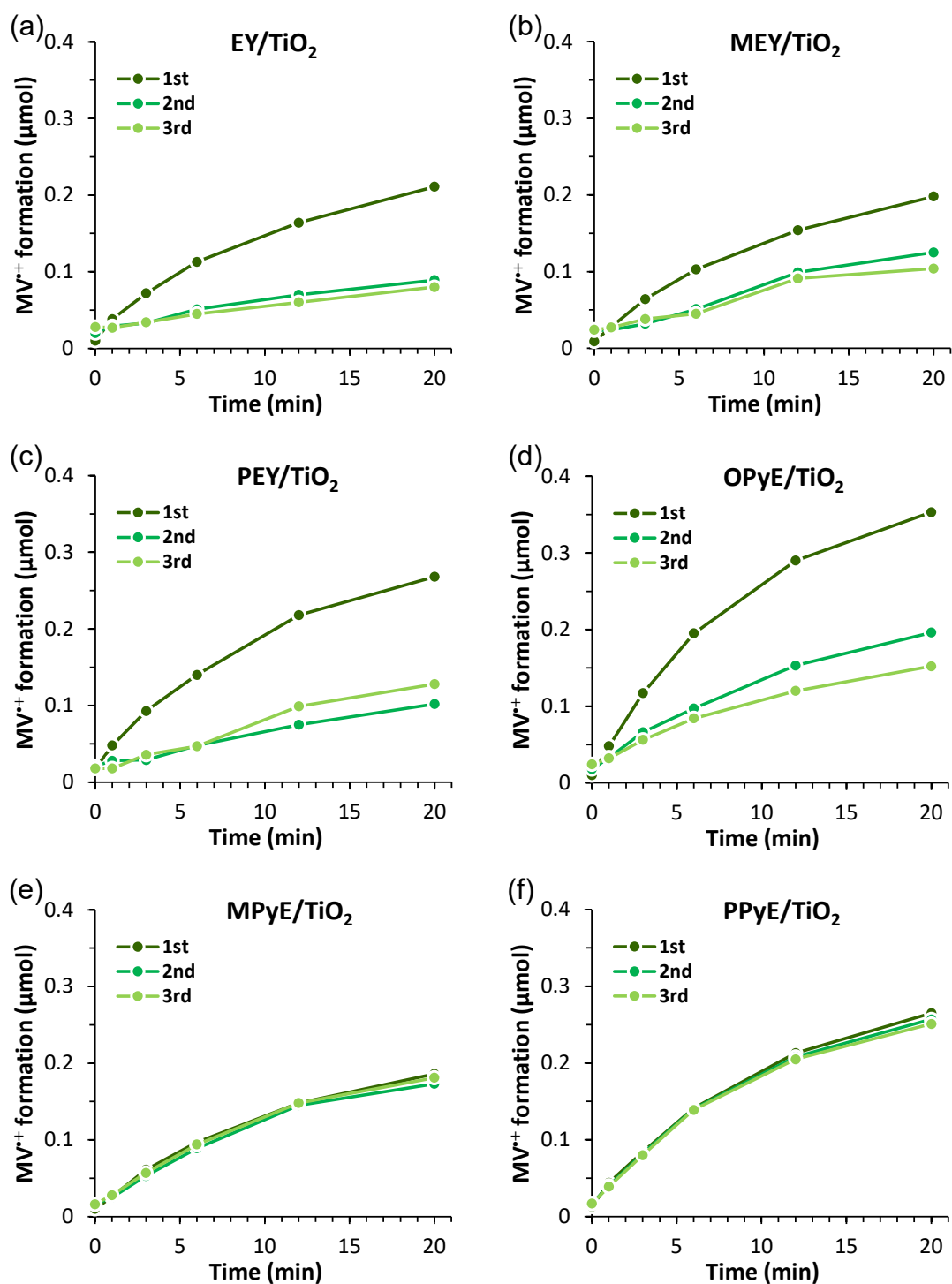


Figure S5. Three-times reusability of different dye/TiO₂ nanoparticles on photocatalytic methyl viologen (MV²⁺) reduction. The reaction mixture consists of 100 mM L-cysteine pH 8, 1 mg/mL dye/TiO₂ composite, 5 mM MV²⁺ solution in total volume of 3 mL under visible light illumination at 520 nm.

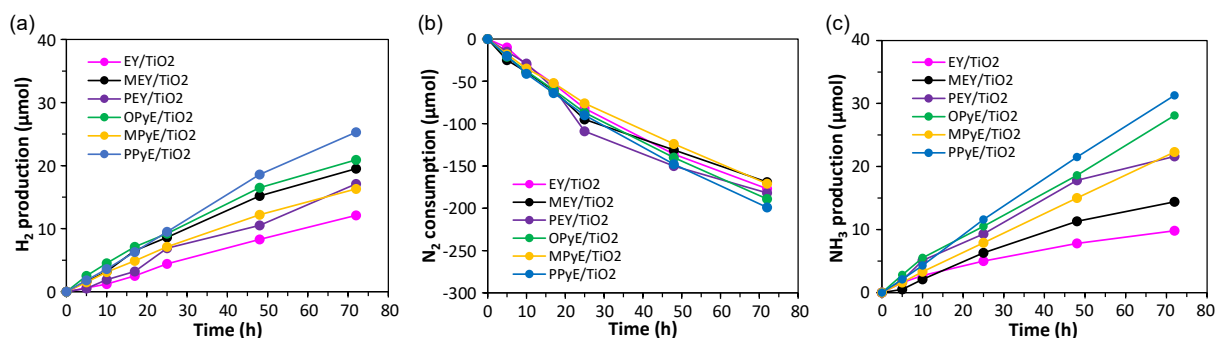


Figure S6. Raw data of (a) H_2 production, (b) N_2 consumption and (c) NH_3 production produced from photobiocatalytic system of dye-modified TiO_2 coupled with cyanobacteria in the reaction system including 100 mM L-cysteine pH 7, 2 mg/mL dye/ TiO_2 , 10 mM MV^{2+} and 50 mg/mL cyanobacterial cell mass under visible light illumination at 520 nm.

Table S10. AQY analysis of NH_3/H_2 production by photobiocatalytic system of dye/ TiO_2 coupled with cyanobacteria.

Dye/TiO ₂	H ₂ production		N ₂ consumption	NH ₃ production	
	Rate (μmol/h)	AQY%	Rate (μmol/h)	Rate (μmol/h)	AQY%
EY/TiO ₂	0.178	0.173	-2.909	0.155	0.229
MEY/TiO ₂	0.319	0.315	-2.705	0.244	0.360
PEY/TiO ₂	0.232	0.227	-3.294	0.364	0.536
OPyE/TiO ₂	0.335	0.329	-2.886	0.376	0.555
MPyE/TiO ₂	0.253	0.248	-2.550	0.312	0.460
PPyE/TiO ₂	0.389	0.382	-3.055	0.452	0.669