Electronic supplementary information for

Platinum-Modified Rod-like Titania Mesocrystals with Enhanced Photocatalytic Activity

Zhishun Wei [1,2], Yuanyuan Ji [1], Zuzanna Bielan [3], Xin Yue [1], Yuqi Xu [1], Jiajie Sun [1], Sha Chen [1,2,*], Guoqiang Yi [1,2], Ying Chang [1,2] and Ewa Kowalska [1,3,*]

[1] Hubei Provincial Key Laboratory of Green Materials for Light Industry, New Materials and Green Manufacturing Talent Introduction and Innovation Demonstration Base, Hubei University of Technology, Wuhan 430068, China; wei.zhishun@hbut.edu.cn (Z.W.); 102100464@hbut.edu.cn (Y.J.); yuexin6912@163.com (X.Y.); 102300431@hbut.edu.cn (Y.X.); sjj73727@163.com (J.S.); yiguoqiang@hbut.edu.cn (G.Y.); cy0025@hbut.edu.cn (Y.C.)
[2] Hubei Longzhong Laboratory, Xiangyang 441000, China
[3] Faculty of Chemistry, Jagiellonian University, 30-387 Krakow, Poland; zuzanna.bielan@uj.edu.pl
* Correspondence: chensha@hbut.edu.cn (S.C.); ewa.k.kowalska@uj.edu.pl (E.K.)

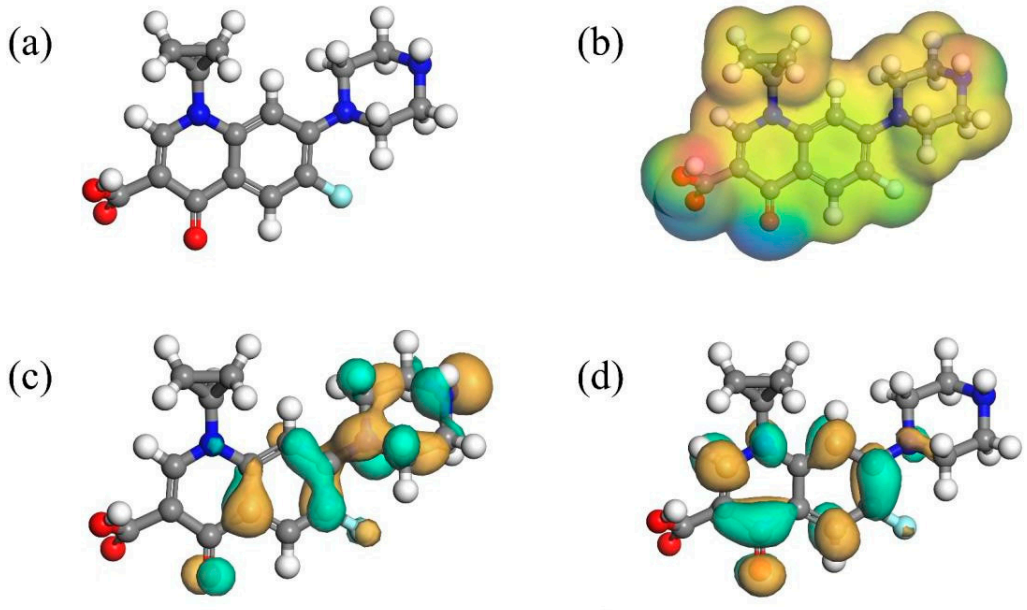

Figure S1. DFT calculations of: (a) optimized structure of CIP; (b) ESP mapping of CIP; (c) the HOMO; and (d) the LUMO distributions in CIP; gray – carbon, red – oxygen, blue – nitrogen, white – hydrogen, cyan – fluorine.

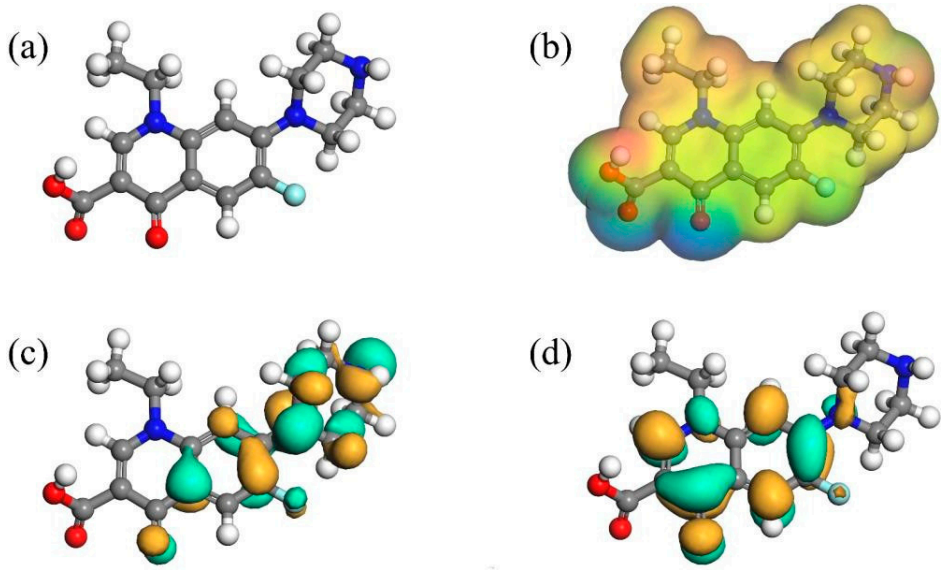

Figure S2. DFT calculations of: (a) optimized structure of NOR; (b) ESP mapping of NOR; (c) the HOMO; and (d) the LUMO distributions in NOR; gray – carbon, red – oxygen, blue – nitrogen, white – hydrogen, cyan – fluorine.

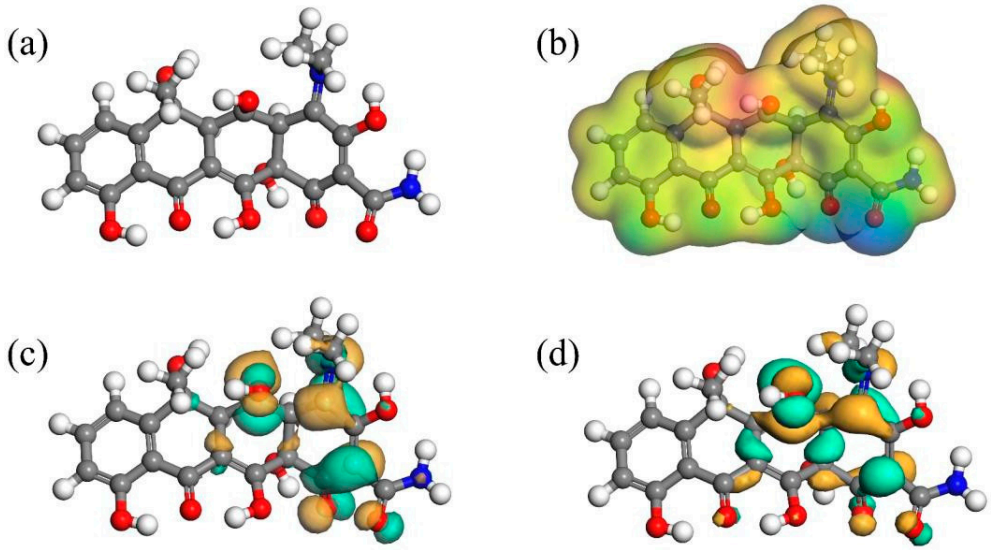

Figure S3. DFT calculations of: (a) optimized structure of OTC; (b) ESP mapping of OTC; (c) the HOMO; and (d) the LUMO distributions in OTC; gray – carbon, red – oxygen, blue – nitrogen, white – hydrogen.

Table S1. Hirshfeld charge and Fukui index values calculated for TC

Atom	q(N)	q(N+1)	q(N-1)	f^-	f^+	f^0
1(C)	0.0293	0.025	0.0399	0.0106	0.0043	0.0074
2(O)	-0.1598	-0.192	-0.1513	0.0085	0.0321	0.0203
3(C)	0.0728	0.0639	0.0742	0.0014	0.0089	0.0052
4(O)	-0.1674	-0.2141	-0.14	0.0274	0.0467	0.0371
5(O)	-0.1923	-0.2299	-0.1319	0.0604	0.0376	0.049
6(O)	-0.2232	-0.295	-0.2057	0.0175	0.0717	0.0446
7(O)	-0.1954	-0.22	-0.1922	0.0032	0.0246	0.0139
8(O)	-0.2385	-0.2706	-0.2101	0.0284	0.0321	0.0302
9(C)	0.1652	0.1574	0.1737	0.0084	0.0078	0.0081
10(O)	-0.278	-0.3009	-0.2533	0.0247	0.0229	0.0238
11(N)	-0.1376	-0.1506	-0.1206	0.0171	0.013	0.015
12(N)	-0.088	-0.0897	0.0317	0.1197	0.0017	0.0607
13(C)	-0.0403	-0.0456	-0.0144	0.0259	0.0053	0.0156
14(C)	-0.0529	-0.0567	-0.0277	0.0252	0.0038	0.0145
15(O)	-0.2181	-0.2311	-0.2105	0.0076	0.013	0.0103
16(C)	0.1298	0.0512	0.1366	0.0068	0.0785	0.0427
17(C)	0.1065	0.0503	0.1202	0.0136	0.0562	0.0349
18(C)	-0.0596	-0.0766	-0.0382	0.0214	0.0171	0.0192
19(C)	0.1323	0.1083	0.138	0.0057	0.024	0.0149
20(C)	-0.0241	-0.0253	-0.0185	0.0055	0.0013	0.0034
21(C)	-0.0187	-0.0218	-0.0149	0.0039	0.0031	0.0035
22(C)	-0.0532	-0.0583	-0.0508	0.0025	0.005	0.0037
23(C)	0.0871	0.0853	0.0884	0.0013	0.0018	0.0015
24(C)	-0.0938	-0.099	-0.0901	0.0036	0.0052	0.0044
25(C)	-0.0587	-0.0914	-0.0228	0.0359	0.0326	0.0343
26(C)	-0.0225	-0.0796	0.0039	0.0264	0.0571	0.0417
27(C)	-0.0641	-0.0888	-0.0172	0.0469	0.0247	0.0358
28(C)	0.0046	-0.0234	0.017	0.0124	0.028	0.0202
29(C)	0.0998	0.0695	0.1307	0.0309	0.0302	0.0306
30(C)	-0.0452	-0.0546	-0.0217	0.0235	0.0094	0.0165
31(C)	0.1308	0.099	0.1312	0.0004	0.0318	0.0161
32(C)	-0.0829	-0.0933	-0.0625	0.0203	0.0104	0.0154
33(H)	0.0445	0.0334	0.0569	0.0125	0.0111	0.0118
34(H)	0.1332	0.1242	0.1407	0.0075	0.009	0.0083
35(H)	0.1401	0.1258	0.1492	0.0091	0.0142	0.0117
36(H)	0.1359	0.1241	0.1496	0.0136	0.0118	0.0127
37(H)	0.1688	0.1581	0.1785	0.0096	0.0107	0.0102
38(H)	0.14	0.1256	0.1544	0.0144	0.0144	0.0144
39(H)	0.1112	0.106	0.1178	0.0067	0.0051	0.0059
40(H)	0.0344	0.0241	0.059	0.0245	0.0103	0.0174
41(H)	0.032	0.0279	0.0533	0.0213	0.0041	0.0127
42(H)	0.0207	0.0125	0.0609	0.0402	0.0082	0.0242
43(H)	0.0317	0.0207	0.0569	0.0253	0.011	0.0181

44(H)	0.0227	0.0231	0.0385	0.0159	-0.0004	0.0077
45(H)	0.0148	0.007	0.0542	0.0395	0.0078	0.0236
46(H)	0.16	0.1486	0.1684	0.0084	0.0114	0.0099
47(H)	0.0284	0.0251	0.0383	0.0099	0.0033	0.0066
48(H)	0.0359	0.0258	0.044	0.0081	0.0101	0.0091
49(H)	0.0311	0.0187	0.0363	0.0051	0.0125	0.0088
50(H)	0.034	0.0251	0.0378	0.0038	0.0088	0.0063
51(H)	0.0353	0.0351	0.038	0.0027	0.0001	0.0014
52(H)	0.0322	0.0217	0.0372	0.005	0.0105	0.0078
53(H)	0.032	0.0203	0.0417	0.0096	0.0117	0.0107
54(H)	0.0513	0.0276	0.0722	0.0209	0.0237	0.0223
55(H)	0.0502	0.0208	0.0699	0.0198	0.0294	0.0246
56(H)	0.0359	0.0169	0.0551	0.0192	0.019	0.0191

Table S2. Hirshfeld charge and Fukui index values calculated for CIP

Atom	q(N)	q(N+1)	q(N-1)	f^-	f^+	f^0
1(C)	0.1982	0.1688	0.2098	0.0115	0.0294	0.0205
2(C)	-0.0588	-0.1007	-0.0233	0.0355	0.0419	0.0387
3(C)	0.1176	0.0658	0.1425	0.0249	0.0518	0.0383
4(C)	-0.033	-0.0395	0.0258	0.0588	0.0065	0.0327
5(C)	-0.0408	-0.0961	-0.0142	0.0266	0.0553	0.0409
6(C)	0.0843	0.042	0.1413	0.057	0.0422	0.0496
7(C)	0.0404	-0.0029	0.0659	0.0256	0.0433	0.0344
8(N)	-0.0728	-0.0874	0.0077	0.0805	0.0146	0.0476
9(C)	-0.0076	-0.0138	0.0069	0.0145	0.0062	0.0103
10(C)	-0.0112	-0.0176	-0.0008	0.0104	0.0064	0.0084
11(N)	-0.1654	-0.1713	-0.1452	0.0202	0.0059	0.013
12(C)	-0.0113	-0.018	0.0001	0.0114	0.0067	0.009
13(C)	-0.0054	-0.0094	0.0081	0.0135	0.004	0.0087
14(C)	-0.0785	-0.1309	-0.0578	0.0207	0.0524	0.0366
15(C)	0.0405	0.0298	0.0698	0.0293	0.0107	0.02
16(N)	-0.001	-0.0327	0.0301	0.0312	0.0316	0.0314
17(C)	0.0371	-0.0737	0.058	0.0209	0.1108	0.0659
18(C)	0.0189	0.0189	0.0193	0.0004	-0.0001	0.0002
19(C)	-0.0652	-0.0793	-0.055	0.0103	0.0141	0.0122
20(C)	-0.0618	-0.0761	-0.0463	0.0155	0.0143	0.0149
21(F)	-0.0947	-0.1279	-0.0512	0.0435	0.0332	0.0384
22(O)	-0.2731	-0.3538	-0.176	0.0971	0.0807	0.0889
23(O)	-0.199	-0.22	-0.1817	0.0174	0.0209	0.0192
24(O)	-0.2703	-0.3261	-0.2365	0.0338	0.0558	0.0448
25(H)	0.0595	0.0324	0.081	0.0215	0.0271	0.0243
26(H)	0.0359	0.0321	0.047	0.0111	0.0038	0.0075
27(H)	0.0232	0.0121	0.0518	0.0286	0.0111	0.0199
28(H)	0.0198	0.0132	0.0336	0.0139	0.0065	0.0102
29(H)	0.0379	0.0253	0.0568	0.0189	0.0126	0.0158
30(H)	0.1067	0.0942	0.1265	0.0198	0.0125	0.0162
31(H)	0.036	0.0238	0.0549	0.0188	0.0122	0.0155
32(H)	0.0185	0.0114	0.0327	0.0142	0.0071	0.0106
33(H)	0.0226	0.0141	0.0495	0.0269	0.0085	0.0177
34(H)	0.0364	0.0336	0.0495	0.0131	0.0028	0.0079
35(H)	0.0347	0.0127	0.0499	0.0152	0.0221	0.0186
36(H)	0.0513	0.0114	0.0687	0.0174	0.0399	0.0286
37(H)	0.0474	0.0297	0.0601	0.0126	0.0177	0.0152
38(H)	0.0485	0.0306	0.0596	0.0111	0.0179	0.0145
39(H)	0.0515	0.0442	0.0557	0.0042	0.0073	0.0058
40(H)	0.0522	0.0437	0.0612	0.009	0.0086	0.0088
41(H)	0.0514	0.0328	0.0673	0.0159	0.0186	0.0173
42(H)	0.1794	0.1543	0.1966	0.0172	0.0251	0.0211

Table S3. Hirshfeld charge and Fukui index values calculated for NOR

Atom	q(N)	q(N+1)	q(N-1)	f^-	f^+	f^0
1(C)	-0.0148	-0.0208	0.0034	0.0183	0.006	0.0121
2(C)	-0.0049	-0.0113	0.0121	0.017	0.0065	0.0117
3(N)	-0.0656	-0.0818	0.0251	0.0907	0.0162	0.0534
4(C)	0.0416	0.0003	0.0649	0.0233	0.0413	0.0323
5(C)	-0.0842	-0.1369	-0.0589	0.0253	0.0527	0.039
6(C)	0.0414	0.0289	0.0693	0.0278	0.0126	0.0202
7(C)	-0.0356	-0.0423	0.0287	0.0643	0.0067	0.0355
8(C)	0.1165	0.0705	0.1393	0.0228	0.046	0.0344
9(C)	-0.059	-0.1025	-0.0317	0.0273	0.0435	0.0354
10(C)	0.198	0.1664	0.2082	0.0101	0.0316	0.0209
11(O)	-0.1996	-0.2213	-0.184	0.0156	0.0217	0.0187
12(O)	-0.2703	-0.3284	-0.2407	0.0297	0.0581	0.0439
13(C)	0.0362	-0.0743	0.0557	0.0195	0.1105	0.065
14(N)	-0.0029	-0.0333	0.0182	0.0211	0.0304	0.0257
15(C)	0.016	0.0073	0.0224	0.0063	0.0087	0.0075
16(C)	-0.0852	-0.0947	-0.078	0.0072	0.0096	0.0084
17(O)	-0.2752	-0.3505	-0.1879	0.0873	0.0752	0.0813
18(C)	-0.0401	-0.0968	-0.0134	0.0267	0.0567	0.0417
19(C)	0.081	0.0352	0.1356	0.0546	0.0458	0.0502
20(F)	-0.0945	-0.129	-0.053	0.0415	0.0345	0.038
21(C)	-0.0024	-0.0083	0.014	0.0164	0.0059	0.0112
22(C)	-0.0157	-0.021	0.0016	0.0172	0.0054	0.0113
23(N)	-0.1645	-0.1739	-0.1323	0.0322	0.0093	0.0208
24(H)	0.0383	0.0232	0.0626	0.0243	0.0151	0.0197
25(H)	0.0162	0.016	0.0302	0.0139	0.0002	0.0071
26(H)	0.0349	0.0203	0.0605	0.0255	0.0146	0.0201
27(H)	0.0374	0.0334	0.0511	0.0138	0.004	0.0089
28(H)	0.0326	0.0094	0.048	0.0154	0.0232	0.0193
29(H)	0.1793	0.1539	0.1952	0.016	0.0254	0.0207
30(H)	0.052	0.0107	0.0694	0.0173	0.0413	0.0293
31(H)	0.047	0.0312	0.0614	0.0143	0.0158	0.0151
32(H)	0.0411	0.0256	0.0475	0.0064	0.0154	0.0109
33(H)	0.0401	0.019	0.0554	0.0153	0.0211	0.0182
34(H)	0.0353	0.0284	0.035	-0.0003	0.0069	0.0033
35(H)	0.0393	0.0303	0.0489	0.0096	0.0091	0.0093
36(H)	0.0597	0.032	0.0815	0.0219	0.0277	0.0248
37(H)	0.0377	0.0345	0.0535	0.0158	0.0032	0.0095
38(H)	0.0369	0.0204	0.0641	0.0272	0.0166	0.0219
39(H)	0.0133	0.0137	0.0269	0.0136	-0.0004	0.0066
40(H)	0.0359	0.0221	0.0592	0.0233	0.0138	0.0186
41(H)	0.1068	0.0947	0.1312	0.0244	0.0121	0.0182

Table S4. Hirshfeld charge and Fukui index calculated for OTC

Atom	q(N)	q(N+1)	q(N-1)	f^-	f^+	f^0
1(C)	0.1009	0.0782	0.1292	0.0283	0.0227	0.0255
2(C)	-0.0552	-0.0902	-0.015	0.0402	0.035	0.0376
3(C)	-0.0258	-0.0772	0.0011	0.0269	0.0514	0.0391
4(C)	-0.066	-0.0862	-0.0202	0.0458	0.0201	0.033
5(C)	0	-0.0267	0.0152	0.0152	0.0266	0.0209
6(C)	-0.0461	-0.0629	-0.0296	0.0166	0.0167	0.0166
7(C)	0.1569	0.1029	0.1672	0.0103	0.054	0.0322
8(C)	-0.034	-0.038	-0.0242	0.0098	0.004	0.0069
9(C)	0.0486	0.0465	0.0639	0.0153	0.0021	0.0087
10(C)	0.0655	0.0624	0.0818	0.0163	0.0032	0.0097
11(C)	0.1447	0.1046	0.1565	0.0118	0.0401	0.0259
12(C)	0.1763	0.1598	0.1808	0.0044	0.0165	0.0105
13(N)	-0.1432	-0.1574	-0.1322	0.0109	0.0143	0.0126
14(O)	-0.2561	-0.2963	-0.2302	0.0259	0.0402	0.033
15(C)	0.0236	0.0159	0.0305	0.0069	0.0077	0.0073
16(C)	-0.0305	-0.032	-0.0269	0.0036	0.0016	0.0026
17(C)	0.048	0.0462	0.0516	0.0036	0.0018	0.0027
18(C)	-0.0249	-0.0274	-0.0215	0.0035	0.0024	0.0029
19(C)	0.0915	0.0899	0.0938	0.0024	0.0016	0.002
20(C)	-0.0973	-0.104	-0.0907	0.0065	0.0067	0.0066
21(O)	-0.215	-0.2227	-0.2058	0.0092	0.0078	0.0085
22(O)	-0.227	-0.2381	-0.2109	0.016	0.0111	0.0136
23(N)	-0.0622	-0.0667	-0.03	0.0322	0.0045	0.0183
24(C)	-0.0338	-0.0419	-0.0232	0.0106	0.0081	0.0093
25(C)	-0.0409	-0.0458	-0.0302	0.0107	0.005	0.0078
26(O)	-0.1633	-0.2094	-0.1416	0.0217	0.0461	0.0339
27(O)	-0.2212	-0.2773	-0.1733	0.0478	0.0561	0.052
28(O)	-0.243	-0.2611	-0.1827	0.0603	0.0182	0.0392
29(O)	-0.2428	-0.2558	-0.178	0.0648	0.013	0.0389
30(O)	-0.2075	-0.27	-0.1785	0.029	0.0626	0.0458
31(O)	-0.1867	-0.2163	-0.1294	0.0573	0.0296	0.0434
32(C)	0.1138	0.0474	0.1231	0.0093	0.0664	0.0379
33(C)	-0.069	-0.0971	-0.0588	0.0102	0.0281	0.0192
34(H)	0.0529	0.0303	0.0753	0.0224	0.0226	0.0225
35(H)	0.0505	0.0239	0.0712	0.0208	0.0266	0.0237
36(H)	0.0375	0.0211	0.0577	0.0202	0.0164	0.0183
37(H)	0.0396	0.0319	0.0469	0.0072	0.0078	0.0075
38(H)	0.0332	0.0229	0.0485	0.0153	0.0103	0.0128
39(H)	0.1341	0.1158	0.1474	0.0133	0.0183	0.0158
40(H)	0.131	0.1232	0.1362	0.0052	0.0079	0.0065
41(H)	0.0334	0.0198	0.0489	0.0155	0.0136	0.0146
42(H)	0.035	0.0239	0.044	0.009	0.011	0.01
43(H)	0.0157	0.0154	0.0197	0.0039	0.0004	0.0021

44(H)	0.0317	0.0239	0.0387	0.0069	0.0079	0.0074
45(H)	0.0282	0.0182	0.0381	0.0099	0.01	0.0099
46(H)	0.0306	0.0207	0.0392	0.0086	0.0098	0.0092
47(H)	0.0358	0.0294	0.0422	0.0063	0.0064	0.0064
48(H)	0.1576	0.1488	0.166	0.0084	0.0089	0.0086
49(H)	0.1429	0.1354	0.152	0.0091	0.0075	0.0083
50(H)	0.0414	0.0281	0.0555	0.0141	0.0133	0.0137
51(H)	0.0399	0.0358	0.0462	0.0063	0.0041	0.0052
52(H)	0.0276	0.0169	0.0475	0.0199	0.0108	0.0153
53(H)	0.0404	0.0259	0.0545	0.0141	0.0145	0.0143
54(H)	0.0363	0.0357	0.0431	0.0068	0.0007	0.0037
55(H)	0.0244	0.0159	0.043	0.0186	0.0085	0.0136
56(H)	0.1414	0.1265	0.1507	0.0093	0.0149	0.0121
57(H)	0.1091	0.103	0.1245	0.0154	0.0061	0.0107
58(H)	0.1273	0.121	0.1435	0.0162	0.0063	0.0112
59(H)	0.1439	0.1334	0.1578	0.0139	0.0105	0.0122

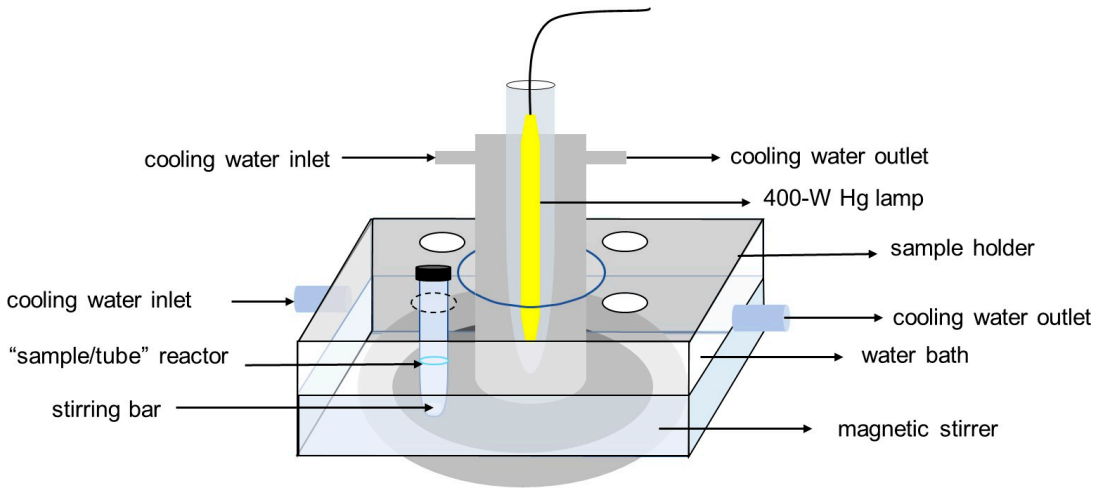

Figure S4. Schematic drawing of photoreactor system used for testing of H_2 evolution reaction.

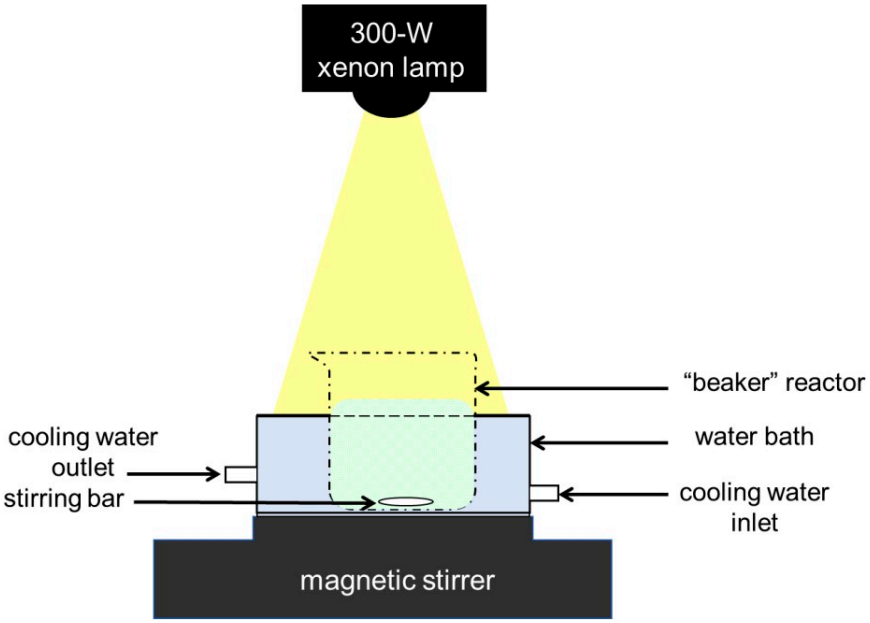

Figure S5. Schematic drawing of photoreactor system used for testing of TC degradation.