Supporting Information

Carbon-Based Binary Organic Photocatalyst for Rapid Dye Degradation under Weak Light: Performance and Mechanistic Study

Ciyuan Huang [a, e], Shasha Shi [a, e], Songlin Cai [a, e], Yue Qiao [a, c], Caiyun Wang [c*], Linji Yang [a], Yuchen Wang [a], Hao Cheng [b*], Tao Yang [d], Kai Huang [c], Bingsuo Zou [a], Tao Liu [a*]

a. C. Huang, S. Shi, S. Cai, Y. Qiao, L. Yang, Prof. B. Zou, Prof. T. Liu,
School of Chemistry and Chemical Engineering, State Key Laboratory of Featured Metal Materials and Life-cycle Safety for Composite Structures, School of Resources, Environment and Materials, Guangxi University, Nanning 530004, China.
Email: liutaozhx@gxu.edu.cn

b. Prof. H. Cheng
Guangxi Key Laboratory of Green Processing of Sugar Resources, College of Biological and Chemical Engineering, Guangxi University of Science and Technology, Liuzhou 545006, Guangxi, P.R. China.
Email: iamchenghao@126.com

c. Y. Qiao, Prof. K. Huang, Prof. C. Wang,
Guangxi Vocational & Technical Institute of Industry, Nanning 530001, China.
Email: wangcaiyun@gxgy.edu.cn

d. Prof. T. Yang.
Centre for Mechanical Technology and Automation, Department of Mechanical Engineering, University of Aveiro, 3810-193 Aveiro, Portugal.

e. These authors contributed equally.

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Table S1. BET surface area and pore diameter of the as-prepared samples.

Samples	S_{BET} (m^2/g)	Pore diameter (nm)
Raw biochar	1190.3	0.7
PM7:ITC-2Cl@C	914.1	0.9
TiO_2@C	301.6	1.9

Table S2. The hole and electron mobility of PM7:ITC-2Cl blend films.

Sample	Hole mobility	electron mobility
PM7:ITC-2Cl	0.000650	0.000390

Table S3. Identified intermediates in the PM7:ITC-2Cl@C system.

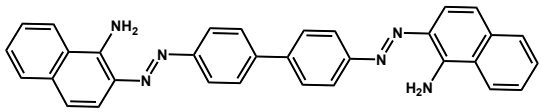
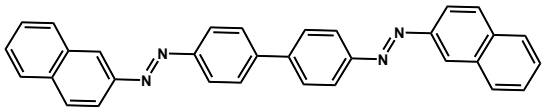
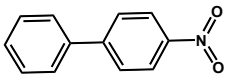
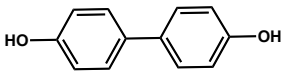
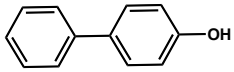
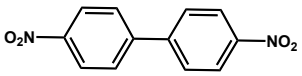
Compound	Formula	MW (g/mol)	Molecular structure
1-Naphthalenamine, 2,2'-[[1,1'-biphenyl]-4,4'-diylbis(2,1-diazenediyl)]bis-	$C_{32}H_{24}N_6$	492.59	
	$C_{32}H_{22}N4$	462.56	
1,1'-Biphenyl, 4-nitro-, radical ion(1-)	$C_{12}H_9NO_2$	199.21	
4,4'-Biphenol	$C_{12}H_{10}O_2$	186.21	
4-Phenylphenol	$C_{12}H_{10}O$	170.21	
4,4'-Dinitrobiphenyl	$C_{12}H_8N_2O_4$	244.21	

Table S4. Ecotoxicity of inter mediate products of Congo red.

	Fish (LC50)	Daphnid (LC50)	Green Algae (EC50)	Fish (ChV)	Daphnid (ChV)	Green Algae (ChV)
CR	5.69	10.2	15.3	0.015	0.169	1.1
DP1	0.0009	0.068	0.050	4.50E-07	0.0017	0.00066
DP2	0.000012	0.000015	0.00027	0.0000029	0.000012	0.00039
DP3	6.3	4.14	5.63	0.732	0.605	2.04
DP4	11.3	7.28	9.22	1.28	1.01	3.22
DP5	3.07	2.37	0.284	0.347	0.324	0.817
DP6	3.34	19.1	2.1	1.63	6.81	0.316

Acute toxicities following the EUP: LC50 >100 or EC50 >100 (Harmless), 10 < LC50 <100 or 10 < EC50 <100 (Harmful), 1< L50 < or 1 < EC50 < 10 (Noxious), and LC50 and LC50 <1 or EC50 < 1 (Very Toxic). At the same time, chronic toxicity according to the national new chemical substance hazard assessment standard (HJ/T154-2004): ChV >10 (Harmless), 1 < ChV < 10 (Harmful), 0.1 < ChV < 1(Toxic), and ChV< 0.1(Very Toxic).

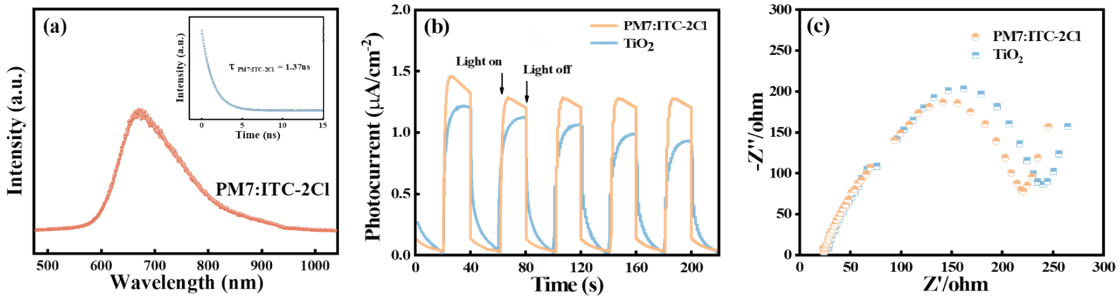


Figure S1. (a) Photoluminescence (PL) spectra and TRPL spectra of PM7:ITC-2Cl. (b) Transient photocurrent responses spectrum (b) and EIS test (c) of PM7:ITC-2Cl blend films and TiO_2.

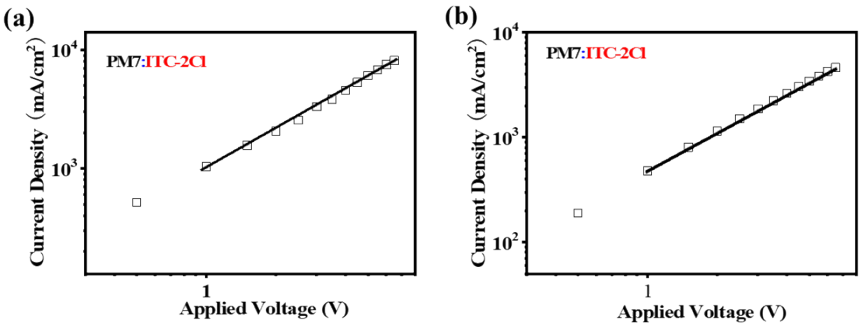


Figure S2. The mobility of hole (a) and electron (b) of PM7:ITC-2Cl blend films.

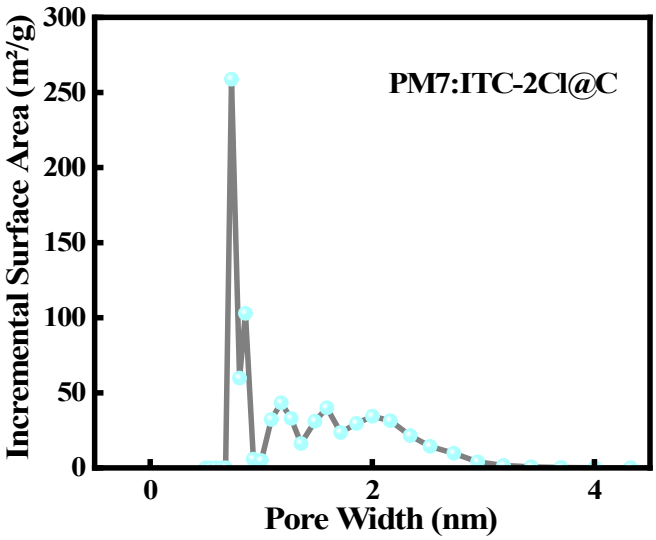


Figure S3. Pore width of PM7:ITC-2Cl@C.

Figure S4. TEM image of PM7:ITC-2Cl blend films.

The uniform surface morphology of PM7:ITC-2Cl can be reflected in the **Figure S2**, which means a highly ordered structure. The blending films of PM7 and ITC-2Cl show obvious self-aggregation region, with quite clear phase separation and interpenetrating network morphology, which provides a continuous seepage path for charge, facilitates exciton dissociation and carrier transport, and thus improves the effective charge separation.

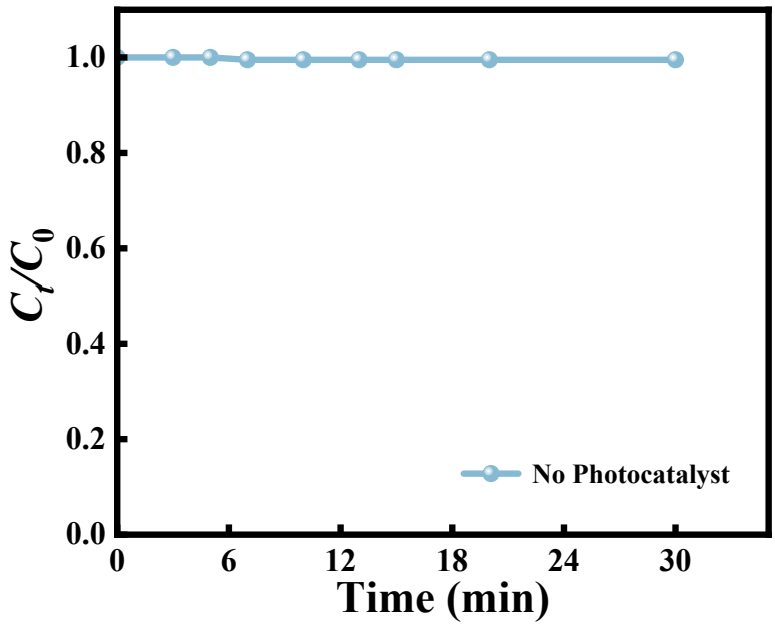
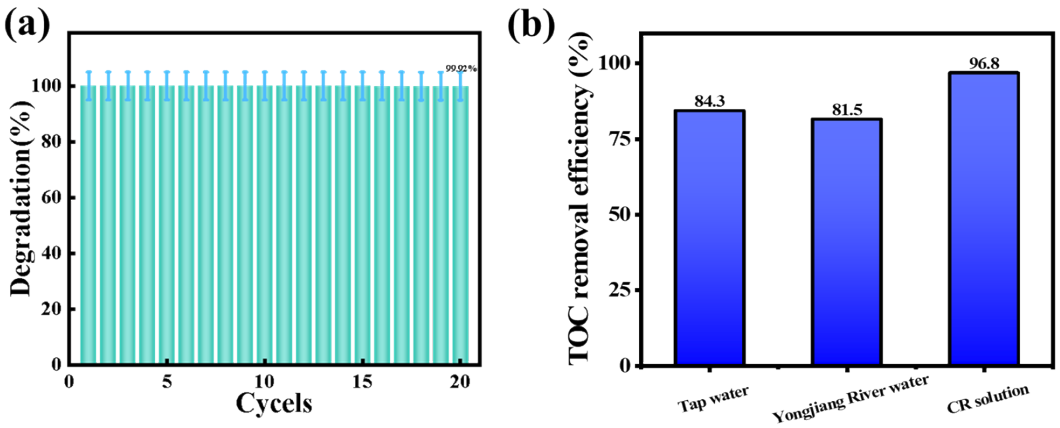


Figure S5. The degradation efficiency of CR under weak light irradiation without photocatalysts.



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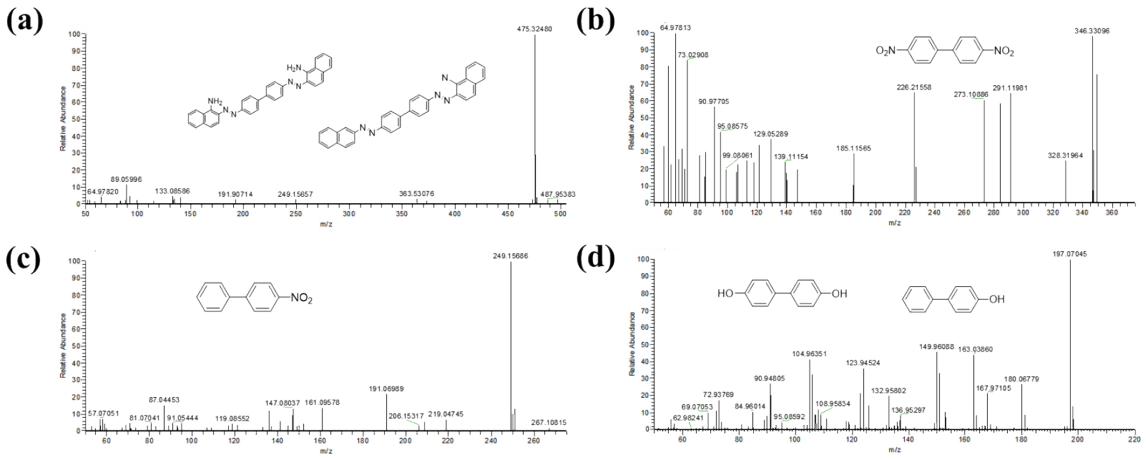


Figure S7. Possible degradation products of CR after irradiation, as determined by LC–MS spectrum.

Figure S8. Natural Population Analysis (NPA) charge distribution on Congo red at different electron state and calculated Fukui index levels.

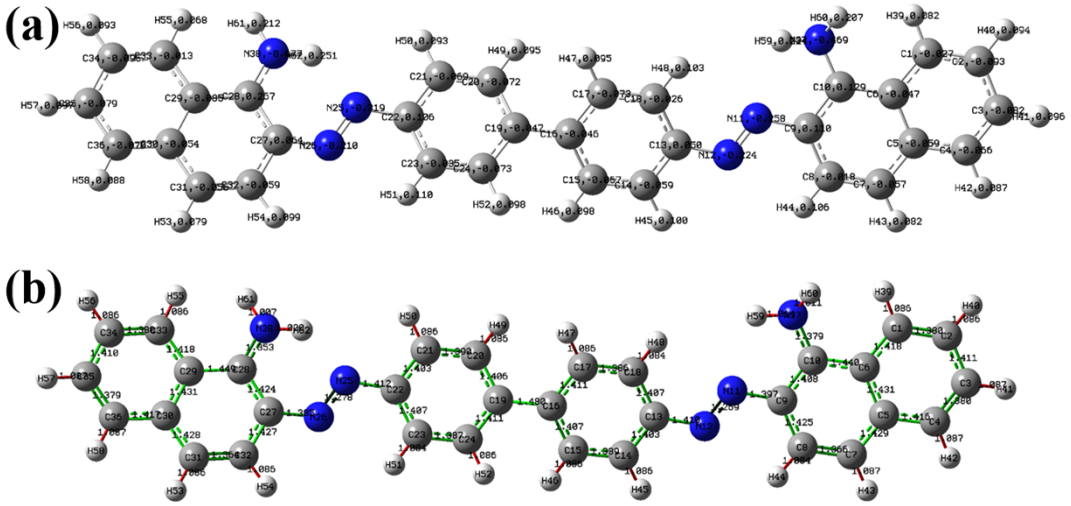


Figure S9. (a) Chemical structure (Mulliken population) of P1. (b) Figure out the bond length of the P1 molecule.

Atom	No	q_N	q_{N+1}	q_{N-1}	f^2	f^+	f^-	f^0
C	1	-0.17645	-0.07942	-0.06008	-0.2134	-0.09703	0.11637	0.00967
C	2	-0.19994	-0.11589	-0.0869	-0.19709	-0.08405	0.11304	0.014495
C	3	-0.18746	-0.08918	-0.07194	-0.2138	-0.09828	0.11552	0.00862
C	4	-0.17672	-0.10058	-0.0664	-0.18646	-0.07614	0.11032	0.01709
C	5	-0.02978	-0.00608	-0.02257	-0.03091	-0.0237	0.00721	-0.008245
C	6	-0.09364	-0.04827	-0.05195	-0.08706	-0.04537	0.04169	-0.00184
C	7	-0.20758	-0.12488	-0.02569	-0.26459	-0.0827	0.18189	0.049595
C	8	-0.18136	-0.07729	-0.11249	-0.17294	-0.10407	0.06887	-0.0176
C	9	0.06204	0.02501	0.09506	0.00401	0.03703	0.03302	0.035025
C	10	0.25183	0.14171	0.17236	0.18959	0.11012	-0.07947	0.015325
N	11	-0.24323	-0.08244	-0.12955	-0.27447	-0.16079	0.11368	-0.023555
N	12	-0.23197	-0.09787	-0.0914	-0.27467	-0.1341	0.14057	0.003235
C	13	0.1187	0.06698	0.0861	0.08432	0.05172	-0.0326	0.00956
C	14	-0.17062	-0.08468	-0.07102	-0.18554	-0.08594	0.0996	0.00683
C	15	-0.19101	-0.09811	-0.08609	-0.19782	-0.0929	0.10492	0.00601
C	16	-0.03646	-0.00673	0.00963	-0.07582	-0.02973	0.04609	0.00818
C	17	-0.18388	-0.1005	-0.08137	-0.18589	-0.08338	0.10251	0.009565
C	18	-0.19384	-0.09129	-0.08546	-0.21093	-0.10255	0.10838	0.002915
C	19	-0.04386	-0.01237	0.0126	-0.08795	-0.03149	0.05646	0.012485
C	20	-0.18865	-0.09531	-0.08696	-0.19503	-0.09334	0.10169	0.004175
C	21	-0.18284	-0.0929	-0.07378	-0.199	-0.08994	0.10906	0.00956
C	22	0.13232	0.07466	0.08994	0.10004	0.05766	-0.04238	0.00764
C	23	-0.19536	-0.09556	-0.08188	-0.21328	-0.0998	0.11348	0.00684
C	24	-0.18002	-0.09605	-0.08204	-0.18195	-0.08397	0.09798	0.007005
N	25	-0.30825	-0.14206	-0.11919	-0.35525	-0.16619	0.18906	0.011435
N	26	-0.20786	-0.06317	-0.12013	-0.23242	-0.14469	0.08773	-0.02848
C	27	0.05337	0.01404	0.10048	-0.00778	0.03933	0.04711	0.04322
C	28	0.24695	0.14284	0.1566	0.19446	0.10411	-0.09035	0.00688
C	29	-0.09697	-0.05044	-0.04628	-0.09722	-0.04653	0.05069	0.00208
C	30	-0.02397	-0.00269	-0.02519	-0.02006	-0.02128	-0.00122	-0.01125
C	31	-0.23309	-0.13914	-0.02317	-0.30387	-0.09395	0.20992	0.057985
C	32	-0.15035	-0.06331	-0.0997	-0.13769	-0.08704	0.05065	-0.018195
C	33	-0.17324	-0.07516	-0.06517	-0.20615	-0.09808	0.10807	0.004995
C	34	-0.20273	-0.11849	-0.0816	-0.20537	-0.08424	0.12113	0.018445
C	35	-0.18472	-0.08609	-0.07701	-0.20634	-0.09863	0.10771	0.00454
C	36	-0.17822	-0.10187	-0.06299	-0.19158	-0.07635	0.11523	0.01944
N	37	-0.76394	-0.38565	-0.30843	-0.8338	-0.37829	0.45551	0.03861
N	38	-0.7356	-0.36245	-0.28613	-0.82262	-0.37315	0.44947	0.03816
H	39	0.19598	0.09397	0.10059	0.1974	0.10201	-0.09539	0.00331
H	40	0.20276	0.09517	0.10799	0.20236	0.10759	-0.09477	0.00641
H	41	0.20306	0.09407	0.10804	0.20401	0.10899	-0.09502	0.006985
H	42	0.20249	0.0959	0.10648	0.2026	0.10659	-0.09601	0.00529
H	43	0.20209	0.09494	0.10617	0.20307	0.10715	-0.09592	0.005615
H	44	0.22648	0.10984	0.11875	0.22437	0.11664	-0.10773	0.004455
H	45	0.21355	0.09991	0.11198	0.21521	0.11364	-0.10157	0.006035
H	46	0.20646	0.09766	0.1075	0.20776	0.1088	-0.09896	0.00492
H	47	0.20395	0.09701	0.10593	0.20496	0.10694	-0.09802	0.00446
H	48	0.21252	0.10214	0.10941	0.21349	0.11038	-0.10311	0.003635
H	49	0.20515	0.09751	0.10704	0.20575	0.10764	-0.09811	0.004765
H	50	0.20578	0.09697	0.10729	0.2073	0.10881	-0.09849	0.00516
H	51	0.2252	0.1079	0.11653	0.22597	0.1173	-0.10867	0.004315
H	52	0.2049	0.09763	0.10707	0.2051	0.10727	-0.09783	0.00472
H	53	0.20406	0.09597	0.10714	0.20501	0.10809	-0.09692	0.005585
H	54	0.2141	0.10238	0.11397	0.21185	0.11172	-0.10013	0.005795
H	55	0.18608	0.08928	0.09596	0.18692	0.0968	-0.09012	0.00334
H	56	0.20308	0.09541	0.10811	0.20264	0.10767	-0.09497	0.00635
H	57	0.20353	0.09424	0.10866	0.20416	0.10929	-0.09487	0.00721
H	58	0.20278	0.09592	0.10668	0.20296	0.10686	-0.0961	0.00538
H	59	0.39228	0.19538	0.19883	0.39035	0.1969	-0.19345	0.001725
H	60	0.369	0.17866	0.19201	0.36733	0.19034	-0.17699	0.006675
H	61	0.3769	0.18143	0.19364	0.37873	0.19547	-0.18326	0.006105
H	62	0.42621	0.21139	0.21401	0.42702	0.21482	-0.2122	0.00131

Figure S10. Calculate the Fukui number per atom of the resulting P1 molecule.

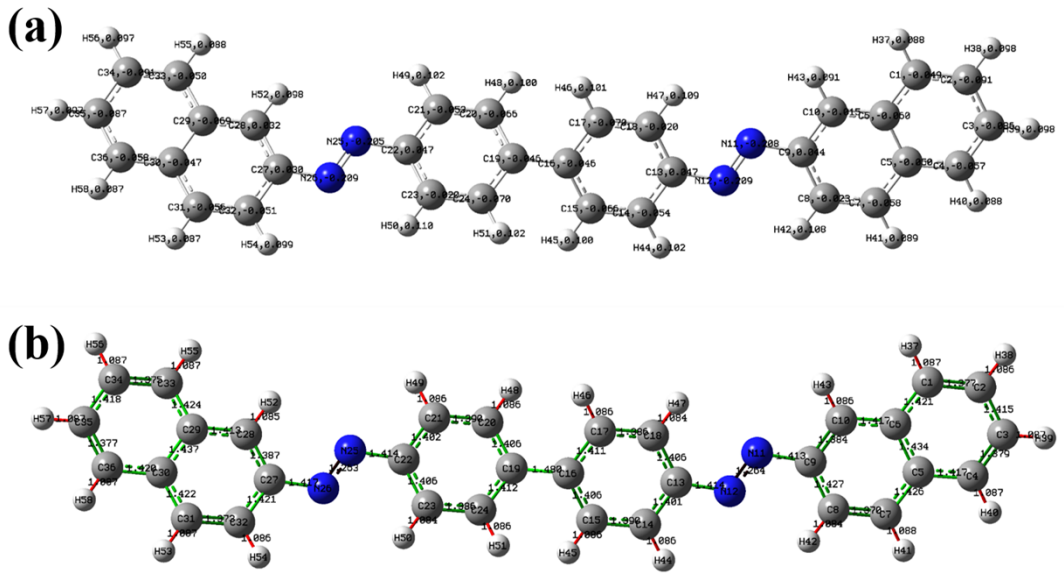
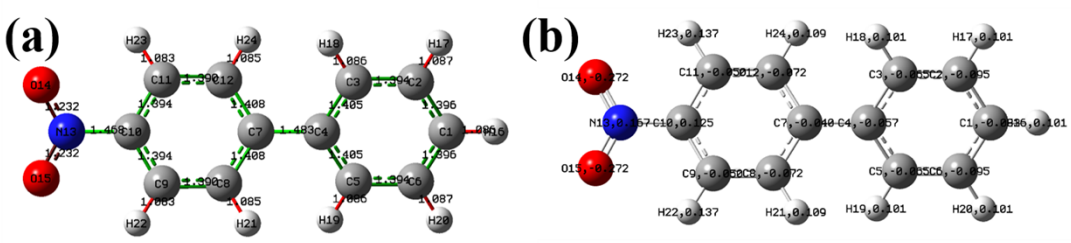


Figure S11. (a) Chemical structure (Mulliken population) of P2. (b) Figure out the bond length of the P2 molecule.

Atom	No	q_N	q_{N+1}	q_{N-1}	f^+	f^-	f^0	f^2
C	1	-0.16742	-0.07547	-0.02474	-0.09195	0.14268	0.025365	-0.23463
C	2	-0.19793	-0.11373	-0.1057	-0.0842	0.09223	0.004015	-0.17643
C	3	-0.18768	-0.09087	-0.03981	-0.09681	0.14787	0.02553	-0.24468
C	4	-0.1786	-0.09956	-0.06683	-0.07904	0.11177	0.016365	-0.19081
C	5	-0.04548	-0.01657	-0.01527	-0.02891	0.03021	0.00065	-0.05912
C	6	-0.06095	-0.03404	-0.04385	-0.02691	0.0171	-0.004905	-0.04401
C	7	-0.16863	-0.10101	-0.04619	-0.06762	0.12244	0.02741	-0.19006
C	8	-0.20063	-0.09033	-0.10953	-0.1103	0.0911	-0.0096	-0.2014
C	9	0.1167	0.06032	0.08833	0.05638	-0.02837	0.014005	0.08475
C	10	-0.14446	-0.05753	0.00694	-0.08693	0.1514	0.032235	-0.23833
N	11	-0.21095	-0.07513	-0.08789	-0.13582	0.12306	-0.00638	-0.25888
N	12	-0.21695	-0.09152	-0.10062	-0.12543	0.11633	-0.00455	-0.24176
C	13	0.11559	0.06395	0.11008	0.05164	-0.00551	0.023065	0.05715
C	14	-0.16772	-0.08376	-0.07276	-0.08396	0.09496	0.0055	-0.17892
C	15	-0.19075	-0.09828	-0.07747	-0.09247	0.11328	0.010405	-0.20575
C	16	-0.03368	-0.00524	0.02368	-0.02844	0.05736	0.01446	-0.0858
C	17	-0.18302	-0.09946	-0.07582	-0.08356	0.1072	0.01182	-0.19076
C	18	-0.186	-0.08894	-0.08334	-0.09706	0.10266	0.0028	-0.19972
C	19	-0.03218	-0.00668	0.02187	-0.0255	0.05405	0.014275	-0.07955
C	20	-0.19123	-0.09842	-0.07618	-0.09281	0.11505	0.01112	-0.20786
C	21	-0.16714	-0.08359	-0.0746	-0.08355	0.09254	0.004495	-0.17609
C	22	0.11454	0.06495	0.10852	0.04959	-0.00602	0.021785	0.05561
C	23	-0.18513	-0.08856	-0.08415	-0.09657	0.10098	0.002205	-0.19755
C	24	-0.18318	-0.10012	-0.07538	-0.08306	0.1078	0.01237	-0.19086
N	25	-0.21101	-0.08721	-0.10405	-0.1238	0.10696	-0.00842	-0.23076
N	26	-0.21154	-0.07326	-0.07842	-0.13828	0.13312	-0.00258	-0.2714
C	27	0.1121	0.05831	0.08805	0.05379	-0.02405	0.01487	0.07784
C	28	-0.16306	-0.05662	0.00358	-0.10644	0.16664	0.0301	-0.27308
C	29	-0.05413	-0.03422	-0.04273	-0.01991	0.0114	-0.004255	-0.03131
C	30	-0.04421	-0.01687	-0.01391	-0.02734	0.0303	0.00148	-0.05764
C	31	-0.17851	-0.10302	-0.04794	-0.07549	0.13057	0.02754	-0.20606
C	32	-0.17943	-0.08522	-0.09758	-0.09421	0.08185	-0.00618	-0.17606
C	33	-0.16858	-0.07259	-0.02087	-0.09599	0.14771	0.02586	-0.2437
C	34	-0.19851	-0.11542	-0.10633	-0.08309	0.09218	0.004545	-0.17527
C	35	-0.18804	-0.0906	-0.03701	-0.09744	0.15103	0.026795	-0.24847
C	36	-0.18	-0.09947	-0.06554	-0.08053	0.11446	0.016965	-0.19499
H	37	0.20322	0.09709	0.10525	0.10613	-0.09797	0.00408	0.2041
H	38	0.20398	0.09605	0.10948	0.10793	-0.0945	0.006715	0.20243
H	39	0.20341	0.09462	0.10755	0.10879	-0.09586	0.006465	0.20465
H	40	0.20276	0.0962	0.10719	0.10656	-0.09557	0.005495	0.20213
H	41	0.20281	0.09549	0.10698	0.10732	-0.09583	0.005745	0.20315
H	42	0.22645	0.11032	0.11761	0.11613	-0.10884	0.003645	0.22497
H	43	0.21332	0.10128	0.10976	0.11204	-0.10356	0.00424	0.2156
H	44	0.21449	0.10008	0.11358	0.11441	-0.10091	0.00675	0.21532
H	45	0.20754	0.09832	0.10851	0.10922	-0.09903	0.005095	0.20825
H	46	0.20628	0.0982	0.10768	0.10808	-0.0986	0.00474	0.20668
H	47	0.2254	0.10758	0.11749	0.11782	-0.10791	0.004955	0.22573
H	48	0.20762	0.09801	0.10847	0.10961	-0.09915	0.00523	0.20876
H	49	0.2144	0.10036	0.11309	0.11404	-0.10131	0.006365	0.21535
H	50	0.22566	0.10744	0.11792	0.11822	-0.10774	0.00524	0.22596
H	51	0.2065	0.09774	0.10803	0.10876	-0.09847	0.005145	0.20723
H	52	0.22331	0.10743	0.11386	0.11588	-0.10945	0.003215	0.22533
H	53	0.20382	0.09526	0.10792	0.10856	-0.0959	0.00633	0.20446
H	54	0.21409	0.10217	0.11311	0.11192	-0.10098	0.00547	0.2129
H	55	0.20349	0.09725	0.1052	0.10624	-0.09829	0.003975	0.20453
H	56	0.20372	0.09558	0.10964	0.10814	-0.09408	0.00703	0.20222
H	57	0.2031	0.09396	0.10769	0.10914	-0.09541	0.006865	0.20455
H	58	0.20238	0.09536	0.10742	0.10702	-0.09496	0.00603	0.20198

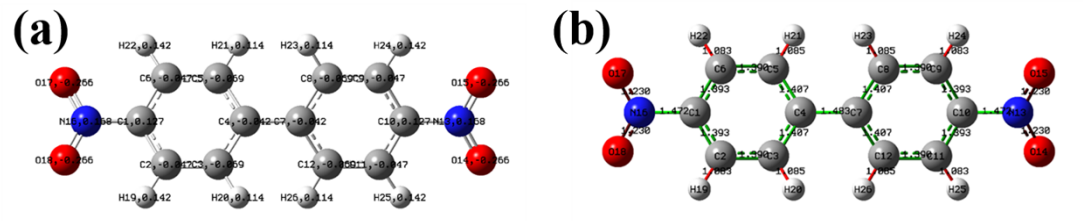
Figure S12. Calculate the Fukui number per atom of the resulting P2molecule.



(c)

Atom	No	q_N	q_{N+1}	q_{N-1}	f^+	f^-	f^0	f^2
C	1	-0.1905	-0.0855	0.11545	-0.105	0.30595	0.100475	-0.41095
C	2	-0.18941	-0.11174	-0.09208	-0.07767	0.09733	0.00983	-0.175
C	3	-0.1848	-0.08211	-0.02468	-0.10269	0.16012	0.028715	-0.26281
C	4	-0.05769	-0.0104	0.11375	-0.04729	0.17144	0.062075	-0.21873
C	5	-0.1848	-0.08211	-0.02468	-0.10269	0.16012	0.028715	-0.26281
C	6	-0.18941	-0.11174	-0.09208	-0.07767	0.09733	0.00983	-0.175
C	7	-0.01062	0.02038	0.05727	-0.031	0.06789	0.018445	-0.09889
C	8	-0.18582	-0.10776	-0.01415	-0.07806	0.17167	0.046805	-0.24973
C	9	-0.17203	-0.07802	-0.10453	-0.09401	0.0675	-0.013255	-0.16151
C	10	0.05805	0.06245	0.18623	-0.0044	0.12818	0.06189	-0.13258
C	11	-0.17203	-0.07802	-0.10453	-0.09401	0.0675	-0.013255	-0.16151
C	12	-0.18582	-0.10776	-0.01415	-0.07806	0.17167	0.046805	-0.24973
N	13	0.50916	0.2962	0.23723	0.21296	-0.27193	-0.029485	0.48489
O	14	-0.38668	-0.19522	-0.15618	-0.19146	0.2305	0.01952	-0.42196
O	15	-0.38669	-0.19522	-0.15618	-0.19147	0.23051	0.01952	-0.42198
H	16	0.20449	0.08902	0.11236	0.11547	-0.09213	0.01167	0.2076
H	17	0.20512	0.09163	0.11915	0.11349	-0.08597	0.01376	0.19946
H	18	0.20567	0.09704	0.11363	0.10863	-0.09204	0.008295	0.20067
H	19	0.20567	0.09704	0.11363	0.10863	-0.09204	0.008295	0.20067
H	20	0.20512	0.09163	0.11915	0.11349	-0.08597	0.01376	0.19946
H	21	0.21289	0.0925	0.11402	0.12039	-0.09887	0.01076	0.21926
H	22	0.23863	0.10761	0.13368	0.13102	-0.10495	0.013035	0.23597
H	23	0.23863	0.10761	0.13368	0.13102	-0.10495	0.013035	0.23597
H	24	0.21289	0.0925	0.11402	0.12039	-0.09887	0.01076	0.21926

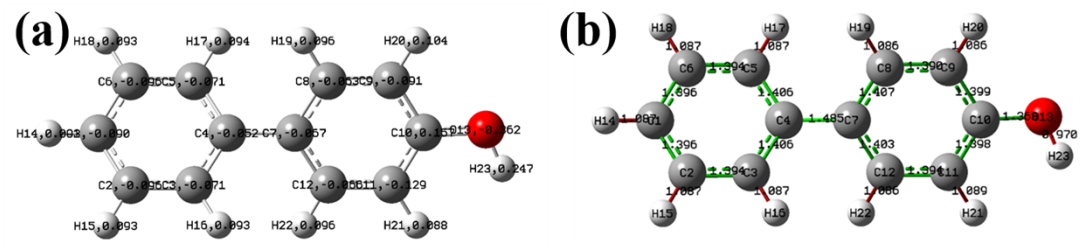
Figure S13. (a) Chemical structure (Mulliken population) of P3. (b) Figure out the bond length of the P3 molecule. (c) Calculate the Fukui number per atom of the resulting P3molecule.



(c)

Atom	No	q_N	q_{N+1}	q_{N-1}	f^+	f^-	f^0	f^2
C	1	0.06568	0.05121	0.20824	0.01447	0.14256	0.078515	-0.12809
C	2	-0.17096	-0.08693	-0.10123	-0.08403	0.06973	-0.00715	-0.15376
C	3	-0.18018	-0.09547	-0.01359	-0.08471	0.16659	0.04094	-0.2513
C	4	-0.0245	0.00679	0.08656	-0.03129	0.11106	0.039885	-0.14235
C	5	-0.18018	-0.09547	-0.01359	-0.08471	0.16659	0.04094	-0.2513
C	6	-0.17096	-0.08693	-0.10123	-0.08403	0.06973	-0.00715	-0.15376
C	7	-0.0245	0.00679	0.08656	-0.03129	0.11106	0.039885	-0.14235
C	8	-0.18018	-0.09547	-0.01359	-0.08471	0.16659	0.04094	-0.2513
C	9	-0.17096	-0.08693	-0.10123	-0.08403	0.06973	-0.00715	-0.15376
C	10	0.06568	0.05121	0.20824	0.01447	0.14256	0.078515	-0.12809
C	11	-0.17096	-0.08693	-0.10123	-0.08403	0.06973	-0.00715	-0.15376
C	12	-0.18018	-0.09547	-0.01359	-0.08471	0.16659	0.04094	-0.2513
N	13	0.50937	0.27953	0.23568	0.22984	-0.27369	-0.021925	0.50353
O	14	-0.38049	-0.19583	-0.15159	-0.18466	0.2289	0.02212	-0.41356
O	15	-0.38049	-0.19583	-0.15159	-0.18466	0.2289	0.02212	-0.41356
N	16	0.50938	0.27953	0.23568	0.22985	-0.2737	-0.021925	0.50355
O	17	-0.38049	-0.19583	-0.15159	-0.18466	0.2289	0.02212	-0.41356
O	18	-0.38049	-0.19583	-0.15159	-0.18466	0.2289	0.02212	-0.41356
H	19	0.24177	0.11122	0.13531	0.13055	-0.10646	0.012045	0.23701
H	20	0.21459	0.09824	0.11586	0.11635	-0.09873	0.00881	0.21508
H	21	0.21459	0.09824	0.11586	0.11635	-0.09873	0.00881	0.21508
H	22	0.24177	0.11122	0.13531	0.13055	-0.10646	0.012045	0.23701
H	23	0.21459	0.09824	0.11586	0.11635	-0.09873	0.00881	0.21508
H	24	0.24177	0.11122	0.13531	0.13055	-0.10646	0.012045	0.23701
H	25	0.24177	0.11122	0.13531	0.13055	-0.10646	0.012045	0.23701
H	26	0.21459	0.09824	0.11586	0.11635	-0.09873	0.00881	0.21508

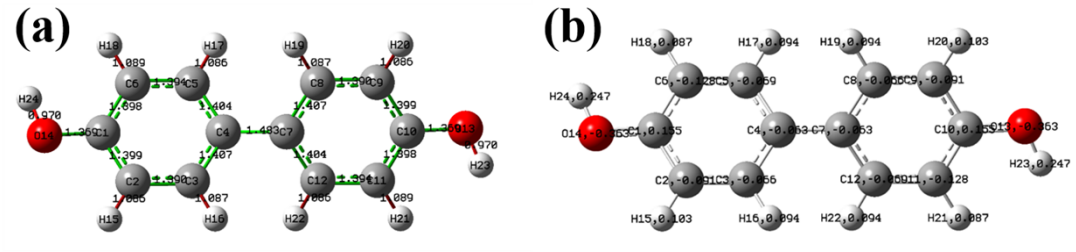
Figure S14. (a) Chemical structure (Mulliken population) of P4. (b) Figure out the bond length of the P4 molecule. (c) Calculate the Fukui number per atom of the resulting P4molecule.



(c)

Atom	No	q_N	q_{N+1}	q_{N-1}	f^+	f^-	f^0	f^2
C	1	-0.2044	-0.04811	0.049	-0.15629	0.2534	0.048555	-0.40969
C	2	-0.19187	-0.11685	-0.10112	-0.07502	0.09075	0.007865	-0.16577
C	3	-0.19439	-0.07983	-0.03215	-0.11456	0.16224	0.02384	-0.2768
C	4	-0.04091	0.0233	0.03398	-0.06421	0.07489	0.00534	-0.1391
C	5	-0.19386	-0.0807	-0.03149	-0.11316	0.16237	0.024605	-0.27553
C	6	-0.19159	-0.11593	-0.10117	-0.07566	0.09042	0.00738	-0.16608
C	7	-0.0778	-0.00928	0.10925	-0.06852	0.18705	0.059265	-0.25557
C	8	-0.1678	-0.06191	-0.05823	-0.10589	0.10957	0.00184	-0.21546
C	9	-0.24995	-0.15558	-0.07491	-0.09437	0.17504	0.040335	-0.26941
C	10	0.33942	0.21707	0.29295	0.12235	-0.04647	0.03794	0.16882
C	11	-0.28282	-0.17416	-0.09826	-0.10866	0.18456	0.03795	-0.29322
C	12	-0.16818	-0.05464	-0.04093	-0.11354	0.12725	0.006855	-0.24079
O	13	-0.66905	-0.34184	-0.21891	-0.32721	0.45014	0.061465	-0.77735
H	14	0.20061	0.07869	0.11086	0.12192	-0.08975	0.016085	0.21167
H	15	0.2006	0.0837	0.11535	0.1169	-0.08525	0.015825	0.20215
H	16	0.20217	0.08733	0.10855	0.11484	-0.09362	0.01061	0.20846
H	17	0.20291	0.08758	0.10908	0.11533	-0.09383	0.01075	0.20916
H	18	0.2008	0.08373	0.11547	0.11707	-0.08533	0.01587	0.2024
H	19	0.20556	0.0908	0.11571	0.11476	-0.08985	0.012455	0.20461
H	20	0.21526	0.09246	0.12345	0.1228	-0.09181	0.015495	0.21461
H	21	0.19861	0.0844	0.11522	0.11421	-0.08339	0.01541	0.1976
H	22	0.20538	0.09018	0.11525	0.1152	-0.09013	0.012535	0.20533
H	23	0.46131	0.21959	0.24304	0.24172	-0.21827	0.011725	0.45999

Figure S15. (a) Chemical structure (Mulliken population) of P5. (b) Figure out the bond length of the P5 molecule. (c) Calculate the Fukui number per atom of the resulting P5molecule.



(c)

Atom	No	q_N	q_{N+1}	q_{N-1}	f^+	f	f^0	f^2
C	1	0.33668	0.14962	0.27396	0.18706	-0.06272	0.06217	0.24978
C	2	-0.24995	-0.10137	-0.0899	-0.14858	0.16005	0.005735	-0.30863
C	3	-0.17104	-0.0556	-0.05447	-0.11544	0.11657	0.000565	-0.23201
C	4	-0.07371	-0.04196	0.06154	-0.03175	0.13525	0.05175	-0.167
C	5	-0.17111	-0.05607	-0.04063	-0.11504	0.13048	0.00772	-0.24552
C	6	-0.28245	-0.11753	-0.11054	-0.16492	0.17191	0.003495	-0.33683
C	7	-0.07371	-0.04196	0.06154	-0.03175	0.13525	0.05175	-0.167
C	8	-0.17104	-0.05561	-0.05447	-0.11543	0.11657	0.00057	-0.232
C	9	-0.24995	-0.10137	-0.0899	-0.14858	0.16005	0.005735	-0.30863
C	10	0.33668	0.14962	0.27396	0.18706	-0.06272	0.06217	0.24978
C	11	-0.28246	-0.11754	-0.11054	-0.16492	0.17192	0.0035	-0.33684
C	12	-0.17111	-0.05607	-0.04063	-0.11504	0.13048	0.00772	-0.24552
O	13	-0.67025	-0.34998	-0.24217	-0.32027	0.42808	0.053905	-0.74835
O	14	-0.67025	-0.34998	-0.24217	-0.32027	0.42808	0.053905	-0.74835
H	15	0.21451	0.08916	0.12206	0.12535	-0.09245	0.01645	0.2178
H	16	0.2039	0.09029	0.11236	0.11361	-0.09154	0.011035	0.20515
H	17	0.20445	0.09068	0.11249	0.11377	-0.09196	0.010905	0.20573
H	18	0.19809	0.08099	0.11384	0.1171	-0.08425	0.016425	0.20135
H	19	0.2039	0.09029	0.11236	0.11361	-0.09154	0.011035	0.20515
H	20	0.21451	0.08916	0.12206	0.12535	-0.09245	0.01645	0.2178
H	21	0.19809	0.08099	0.11384	0.1171	-0.08425	0.016425	0.20135
H	22	0.20445	0.09068	0.11249	0.11377	-0.09196	0.010905	0.20573
H	23	0.46088	0.22179	0.24146	0.23909	-0.21942	0.009835	0.45851
H	24	0.46088	0.22179	0.24146	0.23909	-0.21942	0.009835	0.45851

Figure S16. (a) Chemical structure (Mulliken population) of P6. (b) Figure out the bond length of the P6molecule. (c) Calculate the Fukui number per atom of the resulting P6molecule.

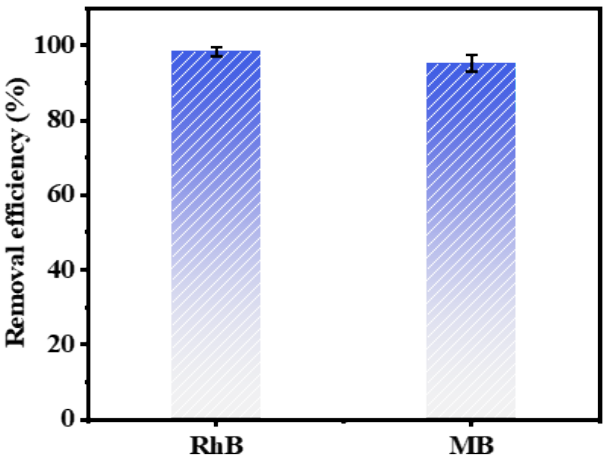


Figure S17. Photocatalytic degradation performance toward other two typical dyeing contaminants: Rhodamine B (RhB) and Methylene blue (MB).