Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information

Theoretical Calculations Based Synthesis of Poly(p-phenylenediamine)-Fe_3O_4 Composite: A Magnetically Recyclable Photocatalyst with Highly Selectivity for Acid Dyes

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Table S1 The surface area and pore structure parameters of Fe_3O_4-PpPD composite

	BET (m^2/g)	Pore volume (mm^3/g)	Pore size (nm)
PdAP	25.58	77.27	12.06

Table S2 The total energy (E_0, Ha), band gap (BG, eV) and the energy (eV) of HOMO-1, HOMO, LUMO, LUMO+1 of PANI (A1) and PpPD (A2-5).

Molecule	total energy (E_0, Ha)	Band Gap (BG, eV)	HOMO-1 (eV)	HOMO (eV)	LUMO (eV)	LUMO+1 (eV)
A1	-1144.301492	1.18745	-5.08965	-5.08965	-3.90220	-3.90220
A2	-682.332765	1.85440	-5.29433	-4.63269	-2.77828	-1.05109
A3	-1021.688234	1.08584	-5.43265	-4.68689	-3.60105	-2.38560
A4	-1021.701963	2.05174	-5.38037	-4.96839	-2.91665	-2.83377
A5	-1361.038991	0.58921	-5.32628	-4.68491	-4.09570	-3.13796

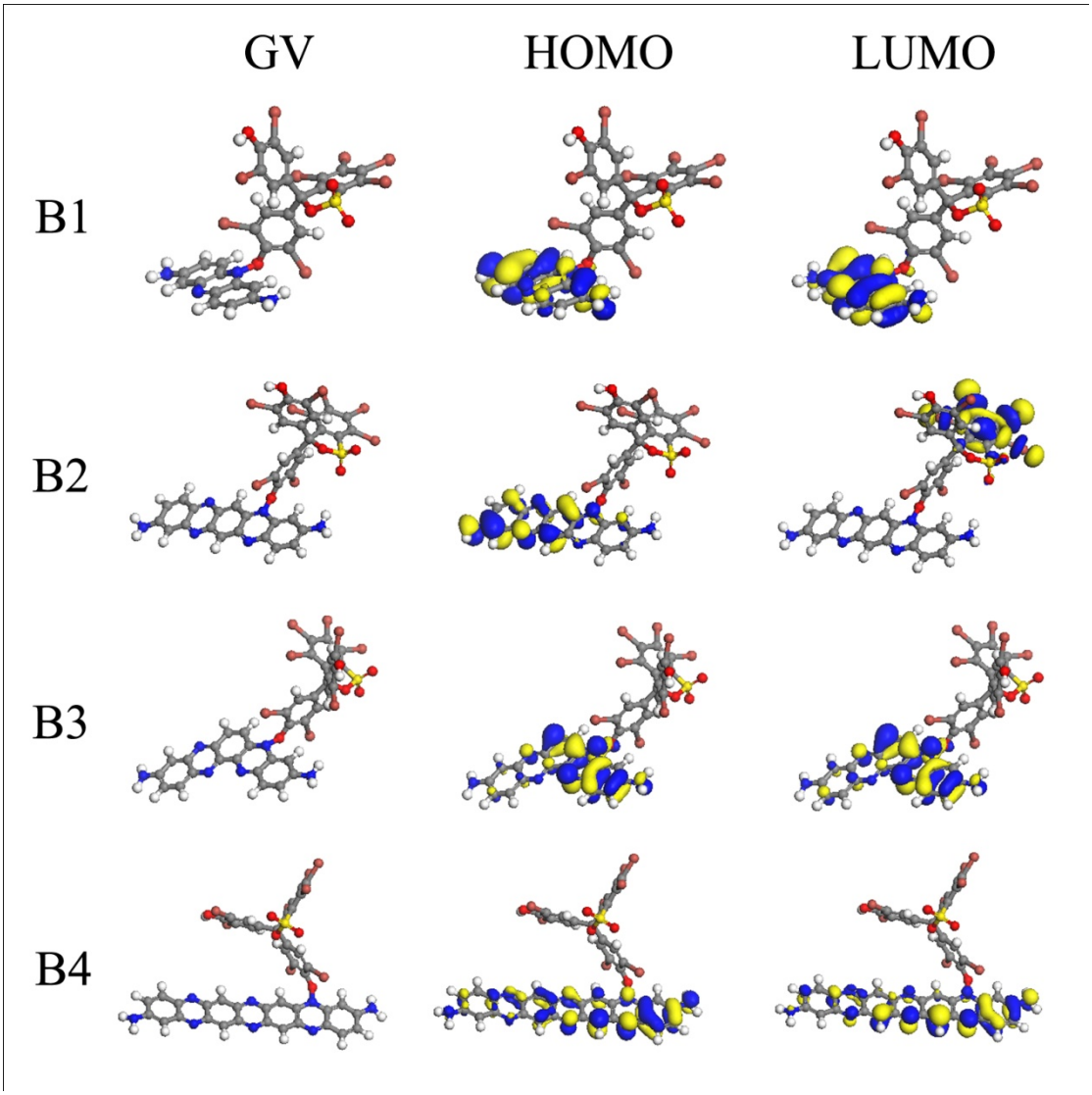


Fig. S1 Ball-and-stick model and theoretical electron dis-tribution of the HOMO–LUMO energy states of B1-4.

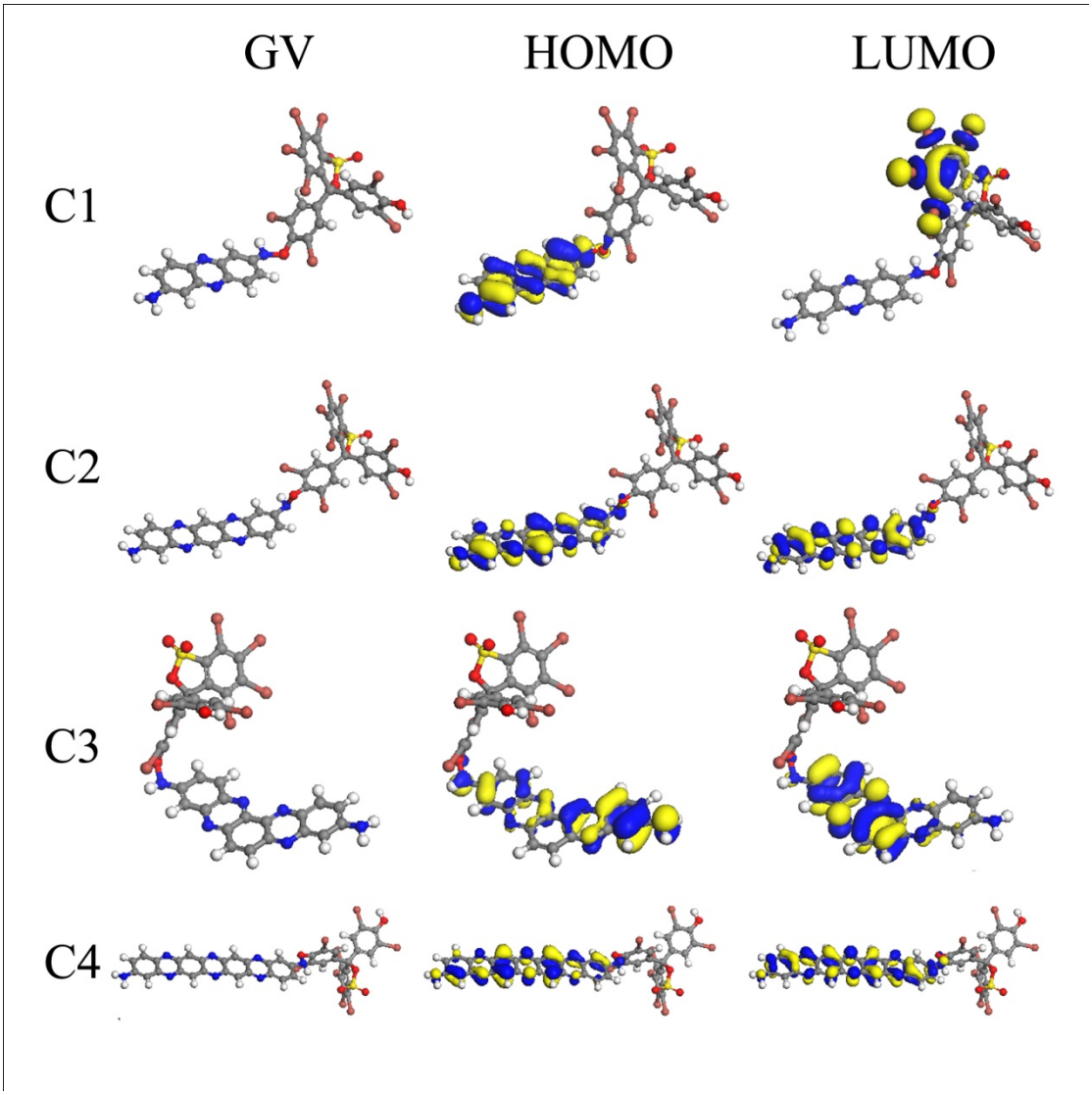


Fig. S2 Ball-and-stick model and theoretical electron dis-tribution of the HOMO–LUMO energy states of C1-4.

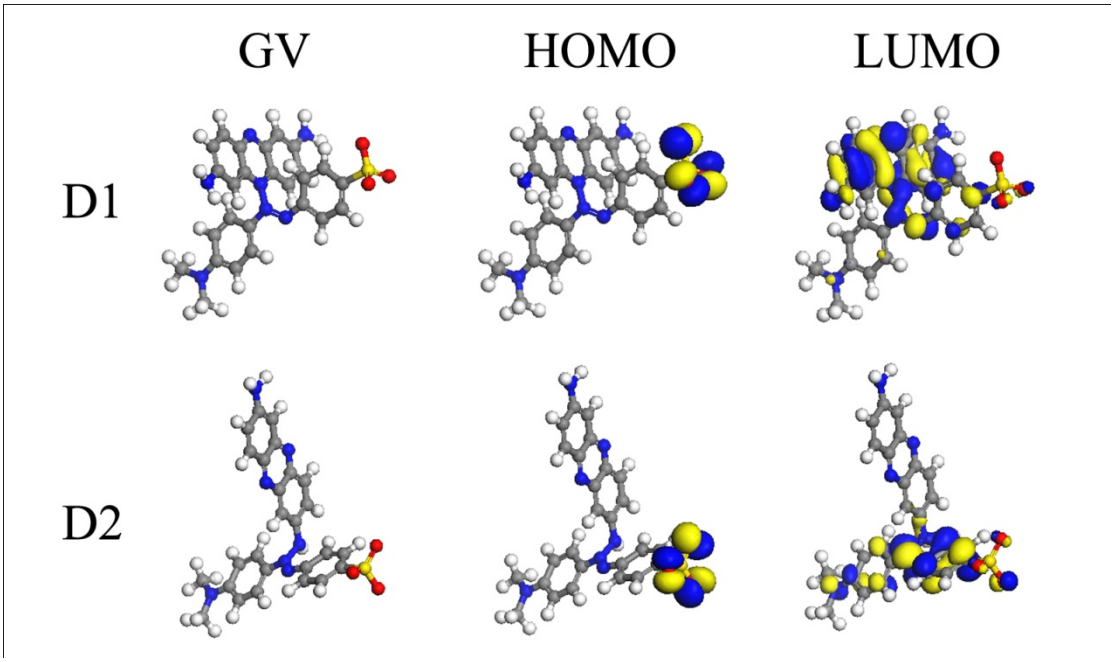


Fig. S3 Ball-and-stick model and theoretical electron dis-tribution of the HOMO–LUMO energy states of D1 and D2.

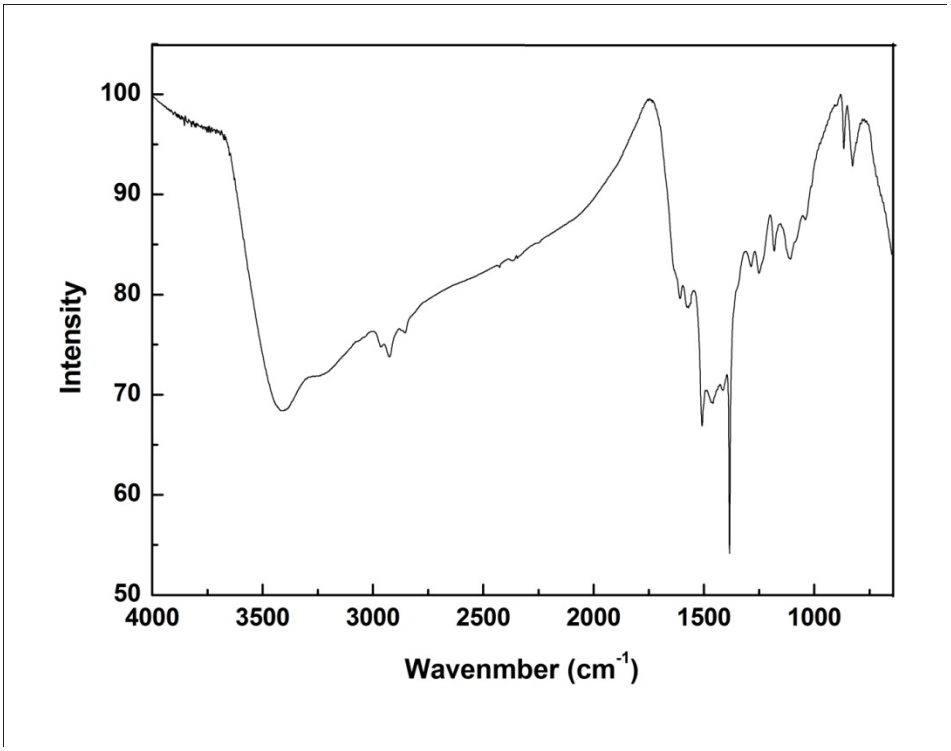
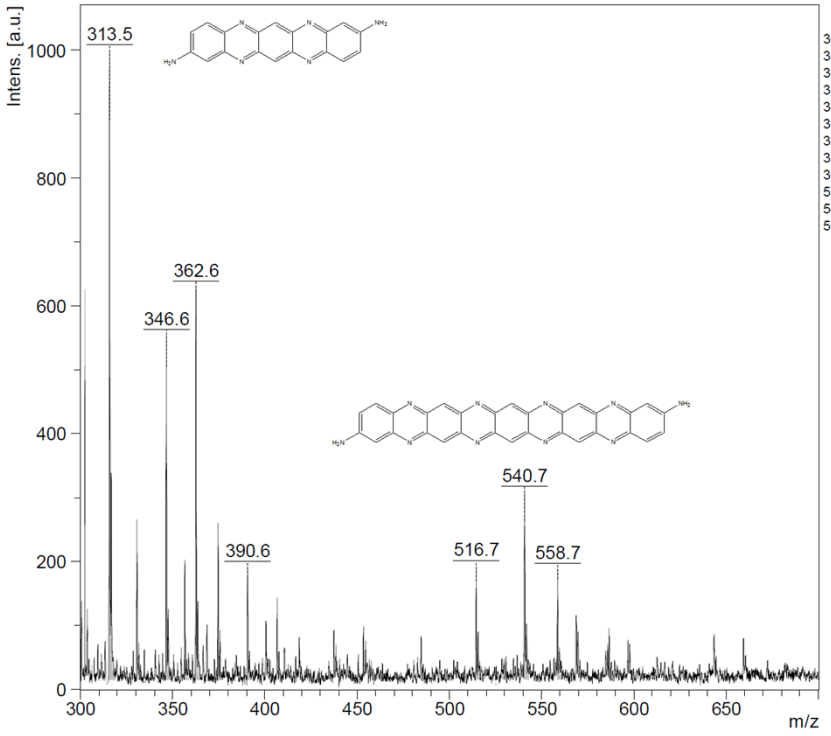


Fig. S4 FT-IR spectra of Fe_3O_4-PpPD composite.



m/z	S/N	Res.	Intens.
302.528	21.4	844	576.75
313.547	34.3	679	887.93
319.484	7.6	1178	210.25
330.567	8.7	883	238.63
346.560	19.2	928	502.24
356.598	6.9	1018	188.60
362.563	23.4	1115	600.47
374.601	9.4	1029	245.48
390.611	6.7	960	178.09
516.720	7.0	1206	166.55
540.748	12.0	1195	260.72
558.654	7.6	1392	169.41

Target

Position	C4

Laser

Laser beam attenuation	98.611
Laser repetition rate	60 Hz
Number of shots	100

Spectrometer

positive voltage polarity	POS
PIE delay	0 ns
Ion source voltage 1	19 kV
Ion source voltage 2	16.85 kV
Lens voltage	5.8 kV
Linear detector voltage	2.667 kV
Deflection on	false
Deflection mass	0 Da
SampleRate	0.5 ns

Instrument

Instrument type	microflex
Serial instrument number	269944.00022
Name of computer	FLEX-PC
Operator ID or name	BDAL@US
flexControl version	flexControl 3.3.99.0
flexAnalysis version	

Date of Acquisition	2011-12-23T03:46:25.531-05:00
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Performed by	Viewed by
Date / Sign	Date / Sign

printed:12/23/2011 3:47:07 AM

Fig. S5 MALDI-TOF-MASS spectrum of PpPD

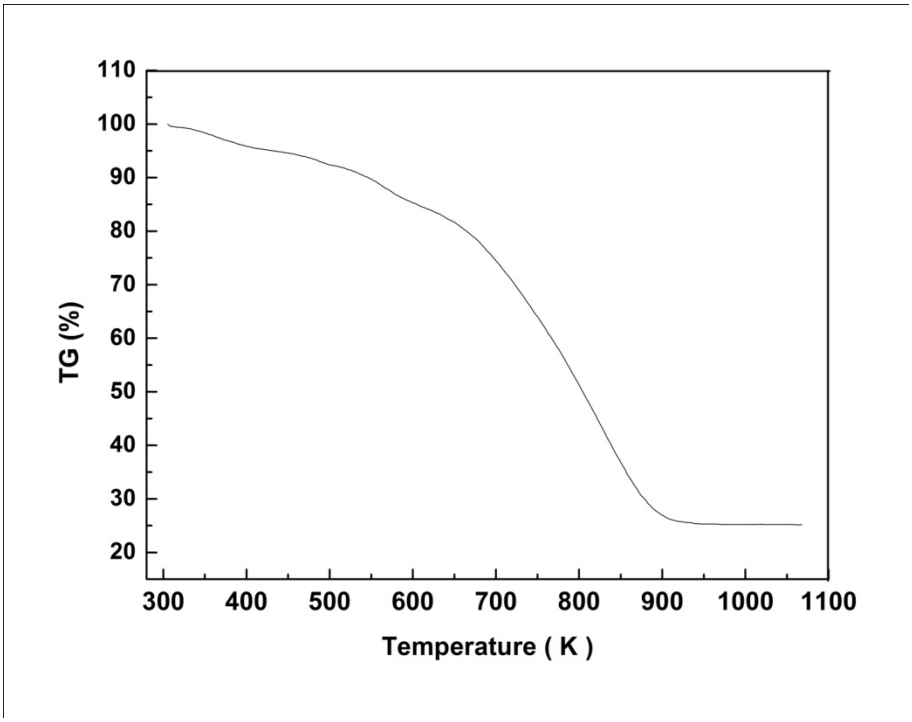

Fig. S6 pectrum of Fe_3O_4-PpPD composite.

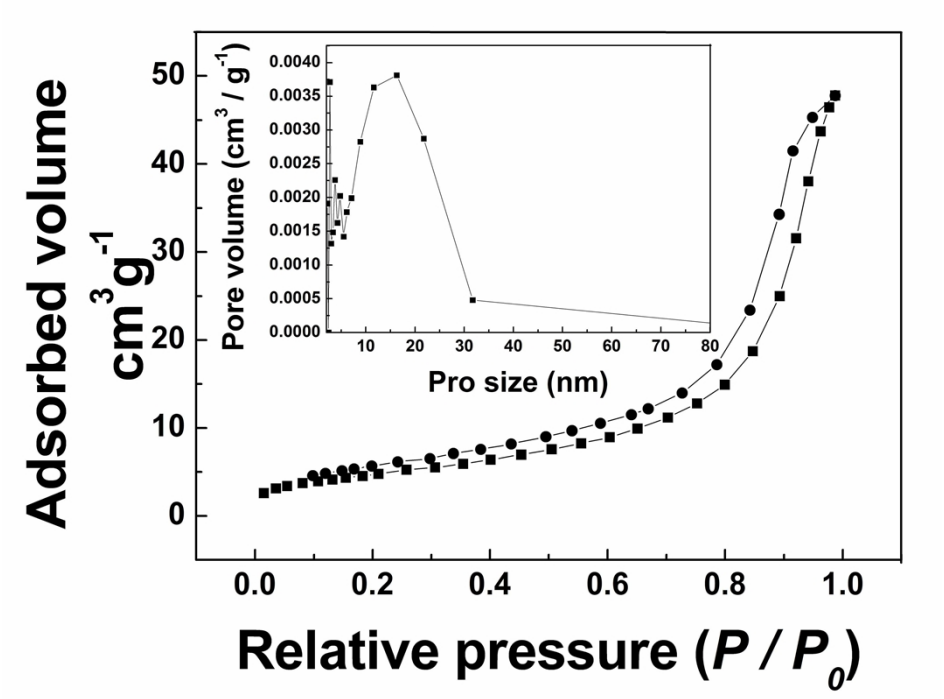

Fig. S7 N_2 adsorption–desorption isotherms of PpPD-Fe_3O_4, the inset shows the pore size distributions of PpPD-Fe_3O_4.

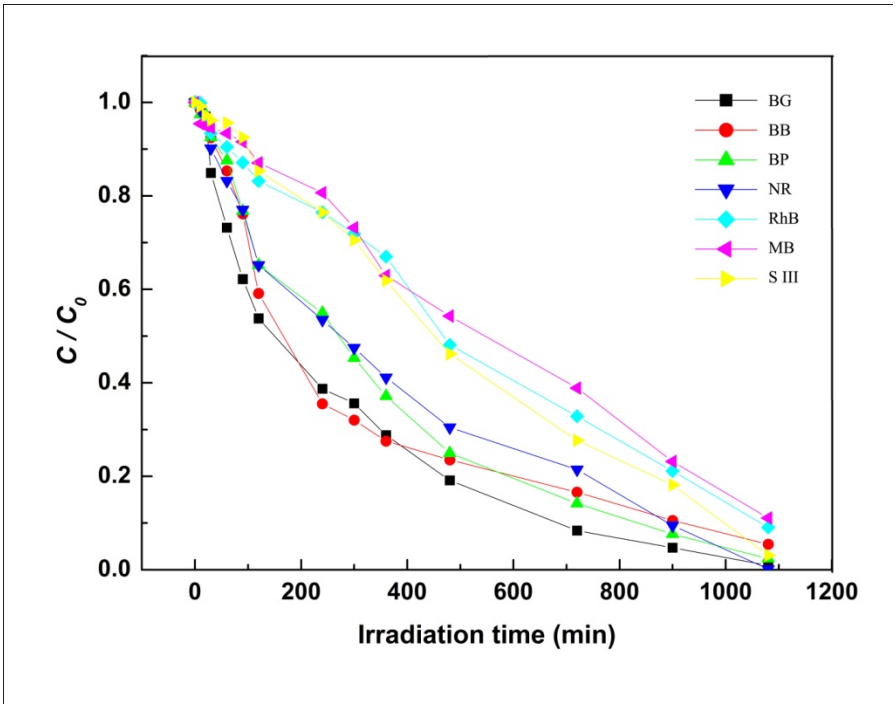

Fig. S8 The photodegradation of dyes under UV ight irradiation.

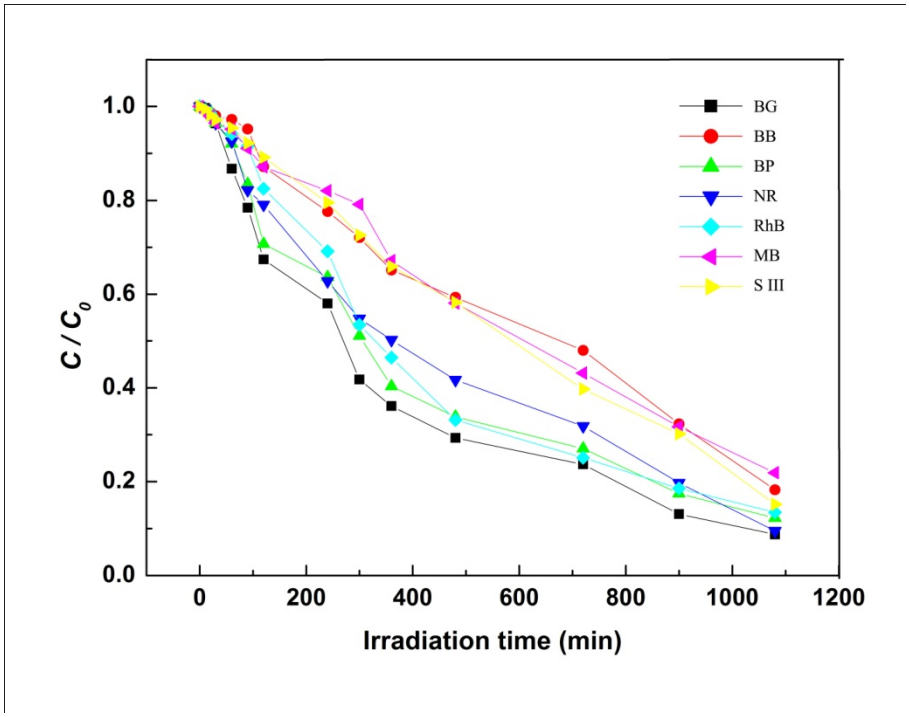

Fig. S9 The photodegradation of dyes under isible light irradiation

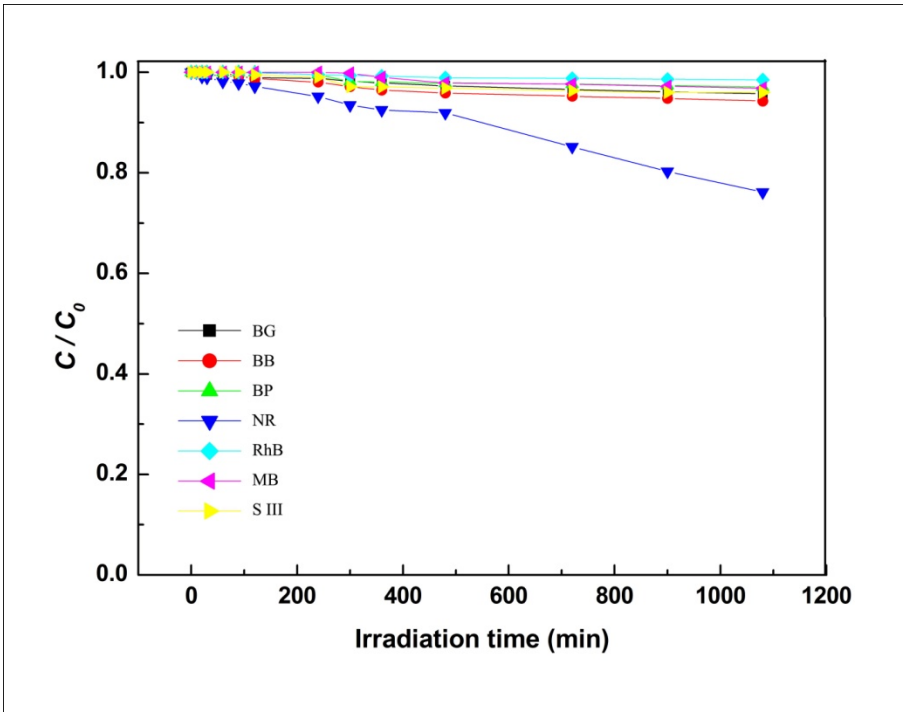

Fig. S10 The photodegradation of dyes in the absent of photocatalysts under UV light irradiation

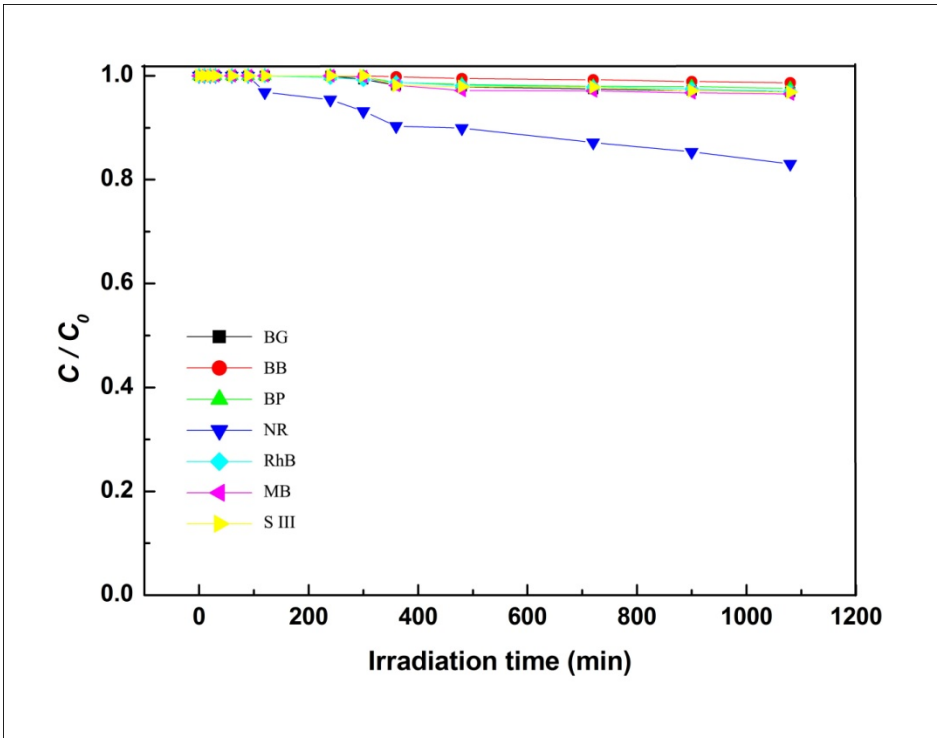

Fig. S11 The photodegradation of dyes in the absent of photocatalysts under visible light irradiation

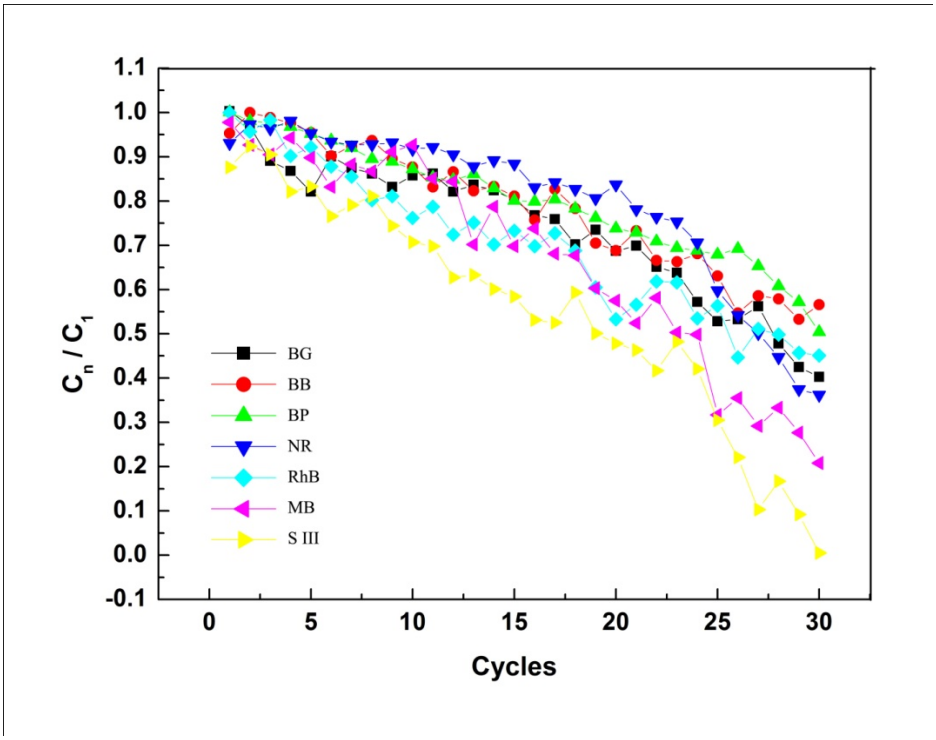

Fig. S12 Photodegradation of dyes in the presence of Fe_3O_4-PpPD under UV light irradiation in 30 cycles

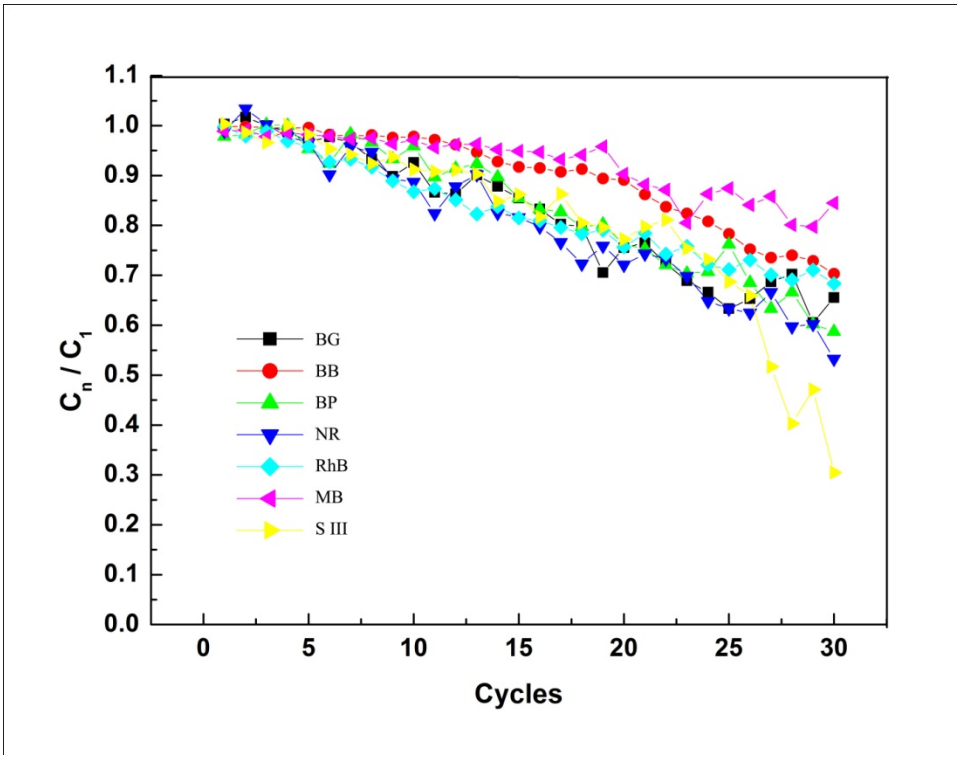

Fig. S13 Photodegradation of dyes in the presence of Fe_3O_4-PpPD unde visible light irradiation in 30 cycles