

Supporting information for:

Synthesis, photocatalytic and antibacterial activities of PDS activated MgO nano-catalyst: Experimental and Theoretical studies

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Table S1: Lattice parameters of MgO NPs

FWHM	2θ	Size (nm)	Average Size(nm)	Dislocation density ($\delta \times 10^{-3}(\text{nm}^{-2})$)	Micro-strain($\epsilon \times 10^{-3}$)
0.35305	18.7312	22.80591	18.60171	1.922671889	9.340019088
0.4251	38.1345	19.77287		2.557764534	5.36640172
0.624259	50.8456	14.09039		5.036791371	5.730519561
0.485165	58.9048	18.80462		2.827943084	3.748929331
0.52948	62.3325	17.53475		3.252377177	3.819822222

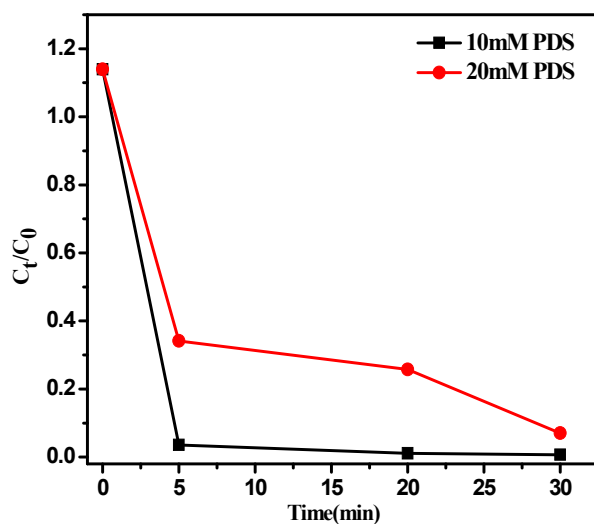


Fig. S1 Different PDS concentration: [MB] =5 mg/L, [MgO] =10mM, pH=9, T= 298.15K)

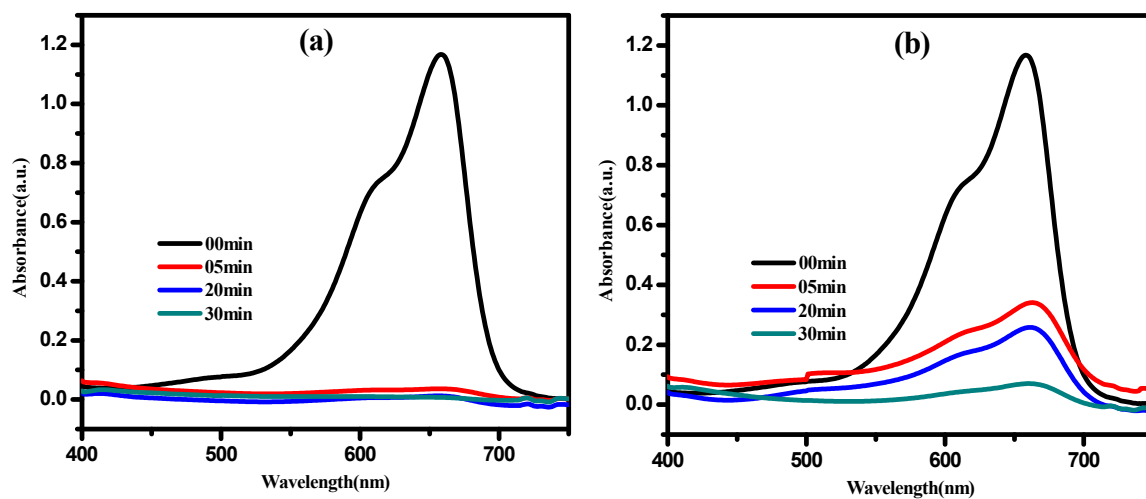


Fig. S2 UV-visible absorption spectra of different PDS concentration with time: (a) [PDS]=10mg/L, [MB] =5 mg/L, [MgO]=10mM, pH=9, T= 298.15K and (b) [PDS]= 20mg/L, [MB] =5 mg/L, [MgO]=10mM, pH=9, T= 298.15K)

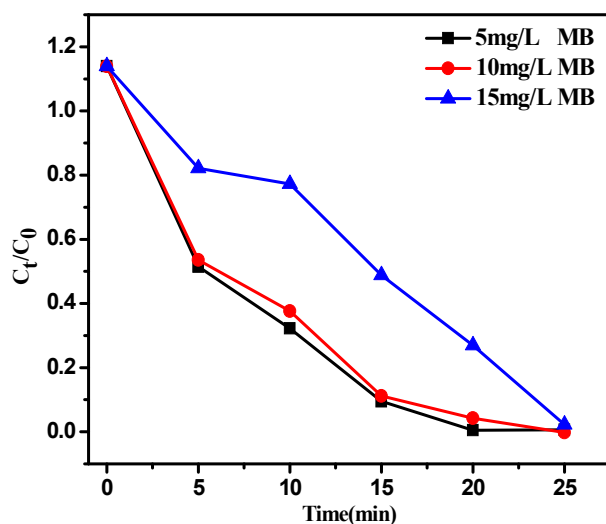


Fig. S3 Different dye concentration: [MgO] =5mM, [PDS]=10mM, pH= 9, T= 298.15K

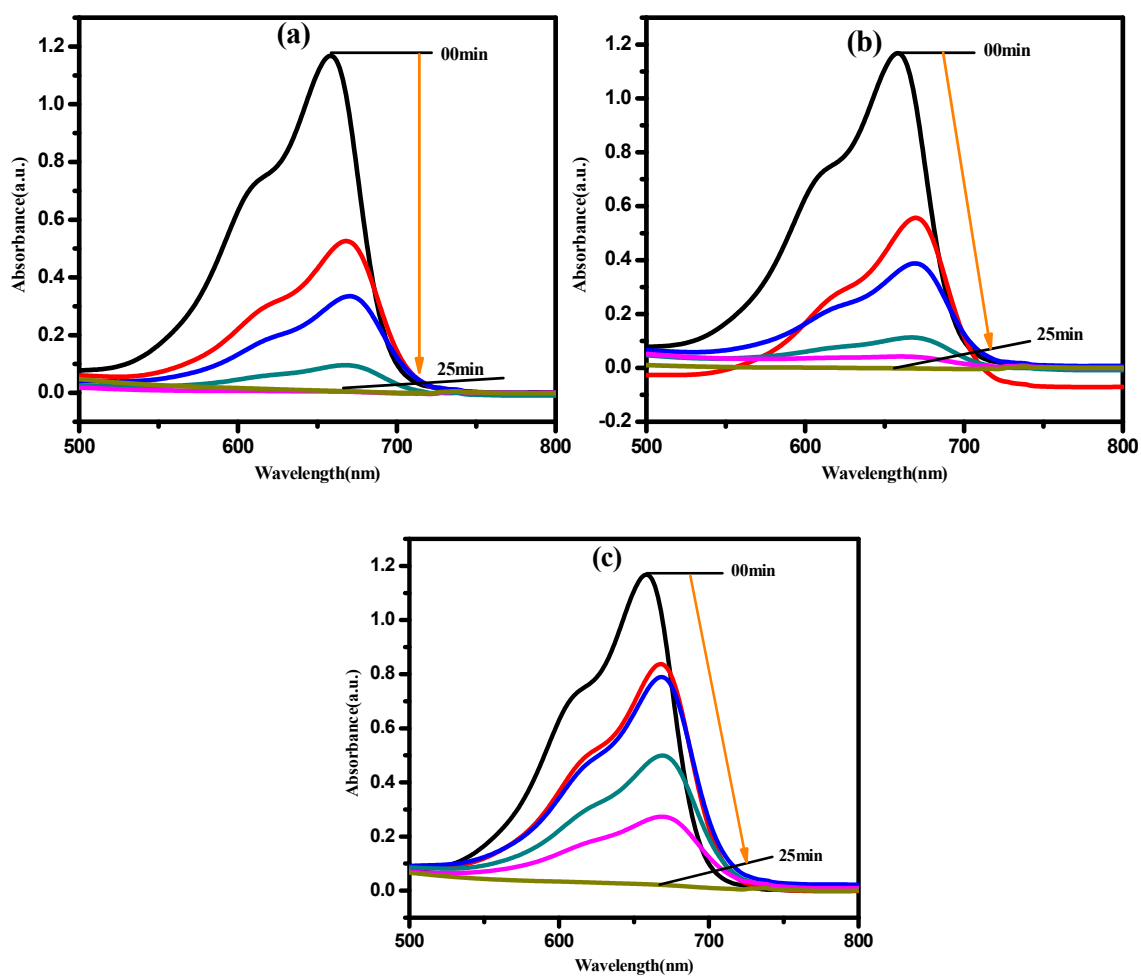


Fig. S4 UV-visible absorption spectra of different dye concentration with time: (a) [MB]=5mg/L, [MgO] =5mM, [PDS]=10mM, pH= 9, T= 298.15K (b) [MB]=10mg/L, [MgO]

=5mM, [PDS]=10mM, pH= 9, T= 298.15K and (c) [MB]=15mg/L, [MgO] =5mM, [PDS]=10mM, pH= 9, T= 298.15K

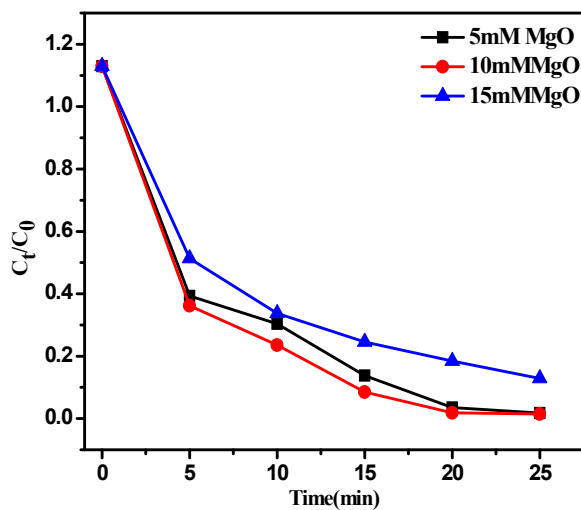
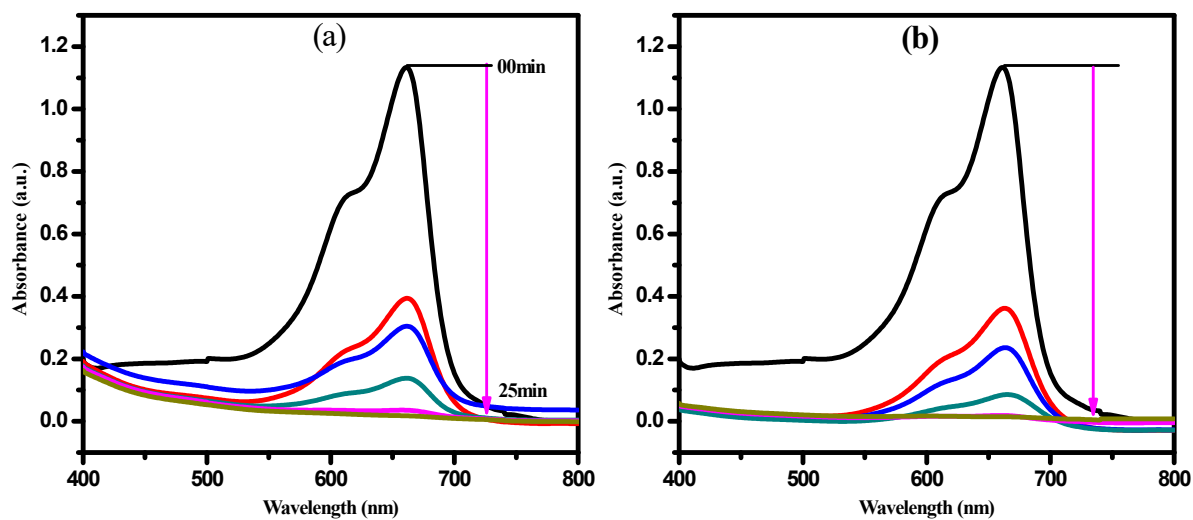


Fig. S5 Different MgO concentration: [MB] =5 mg/L, [PDS] = 10mM, pH= 9, T= 298.15K



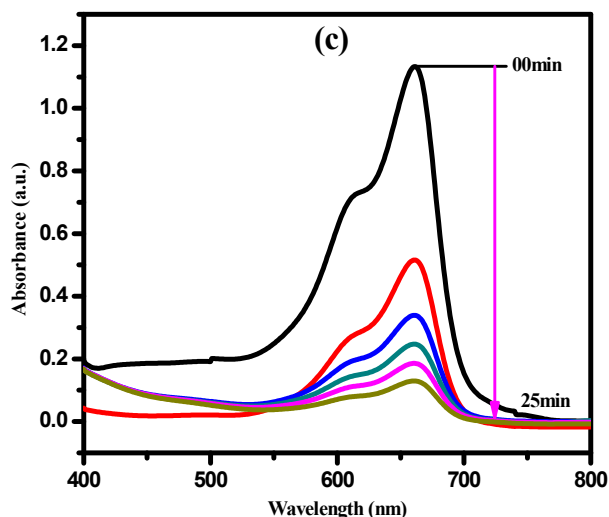


Fig. S6 UV-visible absorption spectra of different catalyst dosage with time: (a) [MB]=5mg/L, [MgO] =5mM, [PDS]=10mM, pH= 9, T= 298.15K (b) [MB]=5mg/L, [MgO] =10mM, [PDS]=10mM, pH= 9, T= 298.15K and (c) [MB]=5mg/L, [MgO] =15mM, [PDS]=10mM, pH= 9, T= 298.15K

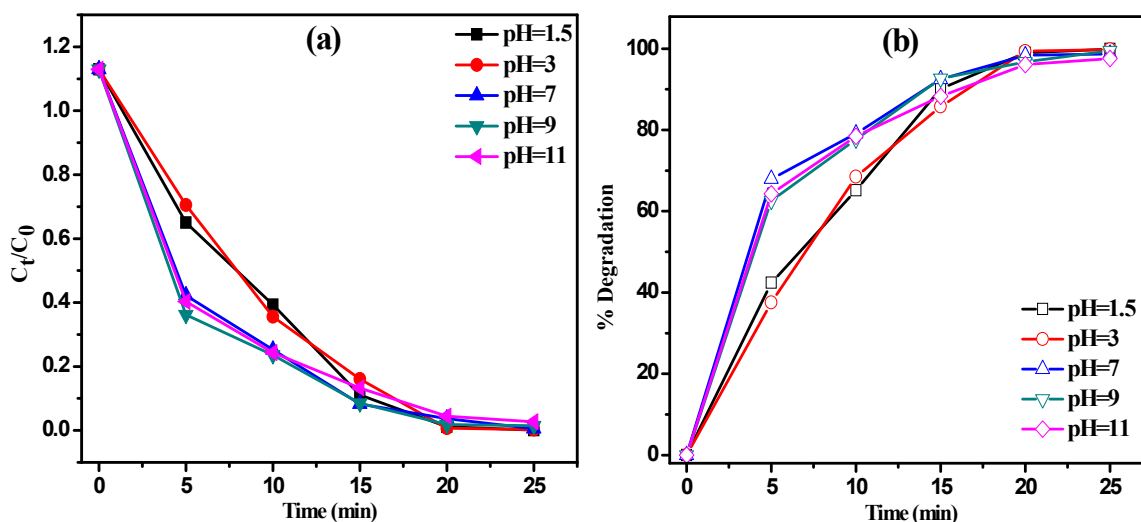


Fig. S7 (a) Different p^H values: [MB] =5 mg/L, [MgO] = 10Mm [PDS]=10Mm, T= 298.15K (b) plot of % degradation with the variation of p^H values from 1.5 to 11

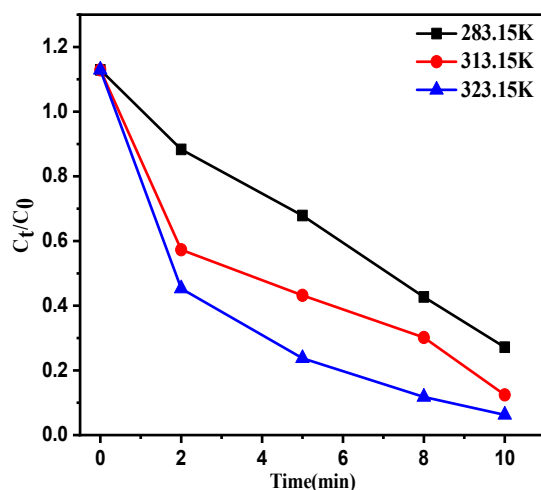


Fig. S8 Different temperatures: [MB] =5 mg/L, [MgO]= 10Mm [PDS]= 10Mm, $p^H=9$

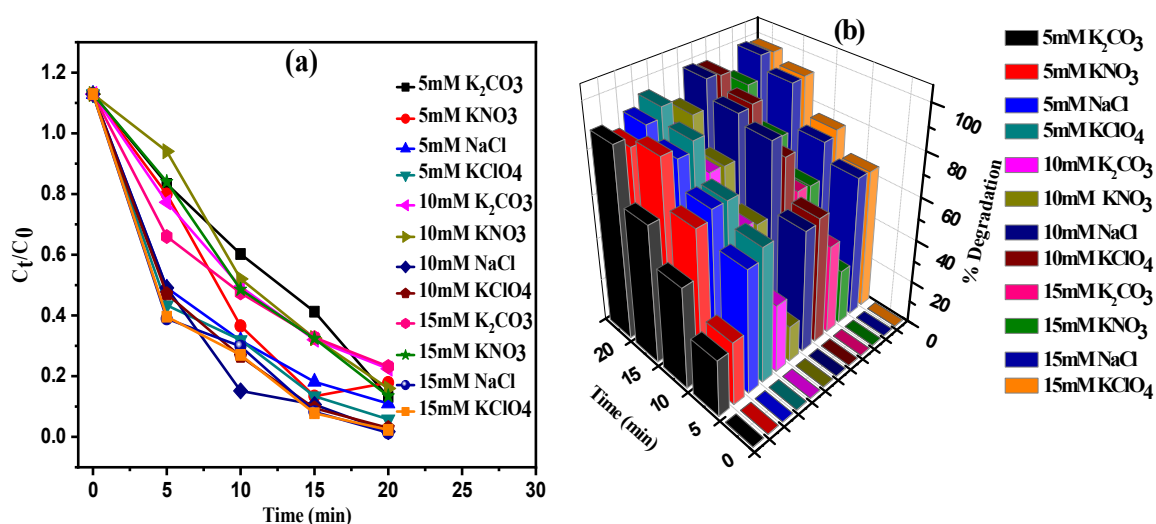


Fig. S9 (a) Different ionic salts ([MB] =5 mg/L, [MgO] =10Mm [PDS] = 10Mm, T= 298.15K) (b) 3D plot of % degradation with the variation of concentration of different salts

Table S2 Kinetic parameters obtained from different kinetic model at different reaction conditions

Parameters	Zero order		1 st Order	
	$k_1(\text{min}^{-1})$	R^2	$k_1(\text{min}^{-1})$	R^2
MgO +MB	0.01977	0.85724	0.76179	0.76179
PDS dosage				

10mM PDS	0.02779	0.19787	0.14577	0.61519
20mM PDS	0.02797	0.49763	0.07756	0.80237
Dye concentration				
5mg/L	0.02779	0.04301	0.23485	0.88265
10mg/L	0.04247	0.81163	0.23567	0.85224
15mg/L	0.04301	0.9775	0.13369	0.68852
Dosage of MgO				
5mM	0.03885	0.70473	0.16503	0.96719
10mM	0.03859	0.65306	0.18076	0.96675
15mM	0.03473	0.7078	0.08136	0.9505
Temperature				
283.15K	0.08318	0.99071	0.13687	0.96402
298.15K	0.043	0.794	0.087	0.95
313.15K	0.08585	0.8079	0.19057	0.90496
323.15K	0.09321	0.7109	0.27223	0.97998
pH value				
pH=1.5	0.04479	0.86283	0.27343	0.89124
pH=7	0.04527	0.87515	0.25718	0.88449
pH=9	0.03966	0.70085	0.19845	0.96102
pH=11	0.03827	0.67707	0.14772	0.9848
Salts				
K ₂ CO ₃	0.7109	0.99325	0.10019	0.86697
KNO ₃	0.05132	0.8557	0.10945	0.84213
NaCl	0.04696	0.76688	0.11308	0.98383
KClO ₄	0.04884	0.76179	0.14222	0.97615