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Supplementary Material

Adsorption-enhanced catalytic wet peroxide oxidation of aromatic compounds on ionothermally synthesised copper-doped magnetite magnetic nanoparticles

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Table S1 Comparison of the particle size and textual properties of undoped Fe_3O_4 and $Fe_{2.88}Cu_{0.12}O_4$ MNPs

Sample	S_{BET} (m^2/g)	V_t (mL/g)	a_0 (Å)[a]	D_{XRD} (nm)[b]	D_{TEM} (nm)[c]
Fe_3O_4	125.0	0.315	8.394	28.3	11.4±3.3
$Fe_{2.88}Cu_{0.12}O_4$	89.4	0.326	8.373	20.3	14.2±2.3

[a] The lattice parameter, a_0, was calculated from the (311) peak by $a_0 = \sqrt{11}d_{311}$.

[b] The average crystallite size, D_{XRD}, was estimated according to the Scherrer equation $D_{XRD} = K\lambda/(\beta\cos\theta)$, where λ is the Cu K_α wavelength, 2θ is the position of the (311) diffraction peak, β is its pure breadth free of the instrumental broadening and K is a constant (0.9 for spherical particles).

[c] The average particle sizes measured from the TEM images.

Table S2 Atom coordinates and single point energies of OG anionic dye and models **1-3** after optimization at B3LYP/6-31G(d) level by DFT .

OG anionic dye (-2048.05067244 a.u.)				Model **1** OG-Cu2+ (-3688.19052206 a.u.)			
Atom	Coordinates (Angstroms)			Atom	Coordinates (Angstroms)		
	X	Y	Z		X	Y	Z
C	3.584223	-0.32396	-0.65943	C	-4.54949	-0.43074	0.372118
C	4.693589	0.460218	-0.31273	C	-5.49745	0.204296	-0.4468
C	5.983211	-0.03055	-0.51418	C	-6.79481	-0.29129	-0.48046
C	6.175345	-1.30541	-1.05416	C	-7.14477	-1.40626	0.290548
C	5.065059	-2.08695	-1.39222	C	-6.19188	-2.03207	1.098137
C	3.77284	-1.59952	-1.20698	C	-4.88694	-1.54986	1.142823
H	4.512295	1.445865	0.104221	H	-5.20082	1.066807	-1.03318
H	6.842877	0.584809	-0.25183	H	-7.53644	0.187796	-1.11314
H	7.182933	-1.68756	-1.21073	H	-8.16058	-1.78979	0.254801
H	5.208516	-3.08591	-1.7998	H	-6.46293	-2.90253	1.687765
H	2.889624	-2.18994	-1.42051	H	-4.11853	-2.02994	1.735692
N	2.24893	0.175012	-0.5919	N	-3.23044	0.056246	0.490975
N	2.079236	0.99744	0.341074	N	-2.86289	1.064575	-0.10034
C	0.803096	1.627746	0.322975	C	-1.62095	1.673925	-0.09618
C	-0.483088	0.983945	0.220144	C	-0.30791	1.068063	0.011169
C	0.894036	3.018356	0.342211	C	-1.74958	3.077084	-0.1837
C	-1.609921	1.835979	-0.083	C	0.792753	1.968252	0.236044
C	-0.775539	-0.40584	0.459605	C	0.017703	-0.31664	-0.13707
C	-0.236862	3.831698	0.129509	C	-0.63549	3.924559	-0.02095
C	-2.891893	1.282024	-0.33402	C	2.102224	1.475657	0.448578
C	-1.453471	3.243714	-0.11593	C	0.595512	3.374962	0.218607
C	-2.048787	-0.89173	0.217947	C	1.308458	-0.76802	0.062071
H	-0.121248	4.916685	0.112271	H	-0.77132	5.002855	-0.05565
C	-3.107304	-0.06773	-0.23878	C	2.343967	0.125762	0.391843
H	-3.724279	1.933088	-0.58522	H	2.91416	2.169604	0.638197
H	-2.328533	3.854405	-0.32733	H	1.455621	4.018079	0.381519
H	-2.25465	-1.92924	0.456393	H	1.514324	-1.82244	-0.08663
O	2.142623	3.603579	0.471977	O	-2.98976	3.587892	-0.35509
H	1.994057	4.56036	0.510958	H	-2.93441	4.556727	-0.3807
S	0.365936	-1.59642	1.294993	S	-1.14501	-1.58085	-0.74505
S	-4.749009	-0.74824	-0.6566	S	3.969663	-0.50263	0.776375
O	1.205991	-2.21585	0.227949	O	-2.06113	-1.82038	0.455778
O	1.12671	-0.74445	2.250339	O	-1.83022	-0.93984	-1.87941
O	-0.549319	-2.56797	1.944969	O	-0.34034	-2.78102	-1.01227
O	-5.067759	-1.67926	0.458132	O	4.310556	-1.50013	-0.33296
O	-4.543683	-1.41451	-1.97228	O	3.966393	-1.05531	2.127052
O	-5.634161	0.452567	-0.72268	O	4.9215	0.684962	0.562769
				Cu	5.939849	-0.44699	-0.66317

Model **2** OG-Fe^{2+} (-3311.50662450 a.u.)				Model **3** OG-Fe^{3+} (-3311.36713411 a.u.)			
Atom	Coordinates (Angstroms)			Atom	Coordinates (Angstroms)		
	X	Y	Z		X	Y	Z
C	-4.46342	-0.42843	0.335219	C	4.384894	-0.11216	-0.2067
C	-5.35215	0.107068	-0.61084	C	4.14146	-1.30471	0.519252
C	-6.63289	-0.42337	-0.70282	C	5.178641	-2.21224	0.65399
C	-7.02284	-1.47541	0.13456	C	6.437288	-1.94248	0.092528
C	-6.1273	-2.00391	1.067946	C	6.674601	-0.7543	-0.61264
C	-4.84007	-1.4857	1.1723	C	5.654187	0.171259	-0.76118
H	-5.02446	0.920442	-1.2486	H	3.157817	-1.48683	0.940207
H	-7.32923	-0.02214	-1.43344	H	5.014334	-3.13785	1.196312
H	-8.02458	-1.88757	0.051874	H	7.239963	-2.6646	0.209202
H	-6.42874	-2.82718	1.708308	H	7.652856	-0.55888	-1.03906
H	-4.11235	-1.89334	1.863065	H	5.801308	1.102373	-1.29803
N	-3.16612	0.095187	0.514385	N	3.422369	0.855692	-0.38051
N	-2.7722	1.069265	-0.1151	N	2.207744	0.735644	-0.23903
C	-1.53772	1.692171	-0.08598	C	1.283449	1.711138	-0.00328
C	-0.22298	1.097447	0.056122	C	-0.09612	1.374086	-0.23191
C	-1.67468	3.091707	-0.20969	C	1.650411	3.019303	0.403852
C	0.871003	2.01172	0.261217	C	-1.07447	2.421983	-0.13807
C	0.109491	-0.28984	-0.04254	C	-0.55052	0.071292	-0.58061
C	-0.56835	3.950983	-0.05642	C	0.662611	4.018786	0.524468
C	2.183122	1.534582	0.489901	C	-2.45912	2.133841	-0.29178
C	0.664869	3.416493	0.204075	C	-0.65169	3.72526	0.249042
C	1.402092	-0.72786	0.175675	C	-1.8469	-0.08235	-1.01489
H	-0.71145	5.027042	-0.11884	H	0.953139	5.022008	0.824757
C	2.429619	0.183823	0.47663	C	-2.83063	0.886281	-0.73459
H	2.989181	2.24276	0.652763	H	-3.20064	2.872569	-0.00176
H	1.519486	4.069782	0.354671	H	-1.40047	4.507261	0.335868
H	1.614499	-1.78577	0.06618	H	-2.14552	-1.0165	-1.47553
O	-2.91665	3.586566	-0.40867	O	2.946038	3.252023	0.628942
H	-2.87049	4.554807	-0.46197	H	3.097166	4.182199	0.873697
S	-1.04498	-1.58519	-0.60154	S	0.192868	-1.53746	-0.07311
S	4.0681	-0.41881	0.86504	S	-4.37916	0.080622	-0.22693
O	-1.97171	-1.76386	0.599432	O	0.875588	-2.17682	-1.189
O	-1.71757	-0.99939	-1.7734	O	0.920197	-1.25231	1.1699
O	-0.2331	-2.79289	-0.8052	O	-1.11977	-2.3393	0.296088
O	4.328765	-1.59579	-0.08332	O	-4.32458	-1.28948	-0.90684
O	4.140995	-0.71793	2.289686	O	-5.54441	0.923294	-0.37228
O	5.046704	0.649639	0.354046	O	-3.96295	-0.32722	1.216406
Fe	5.878849	-0.65099	-0.99299	Fe	-2.93345	-1.91243	0.562353

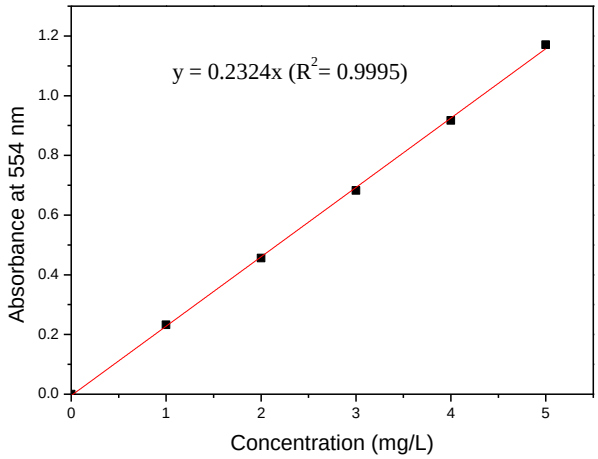

Fig. S1. The standard curve of the RhB concentration and its absorbance at 554 nm.

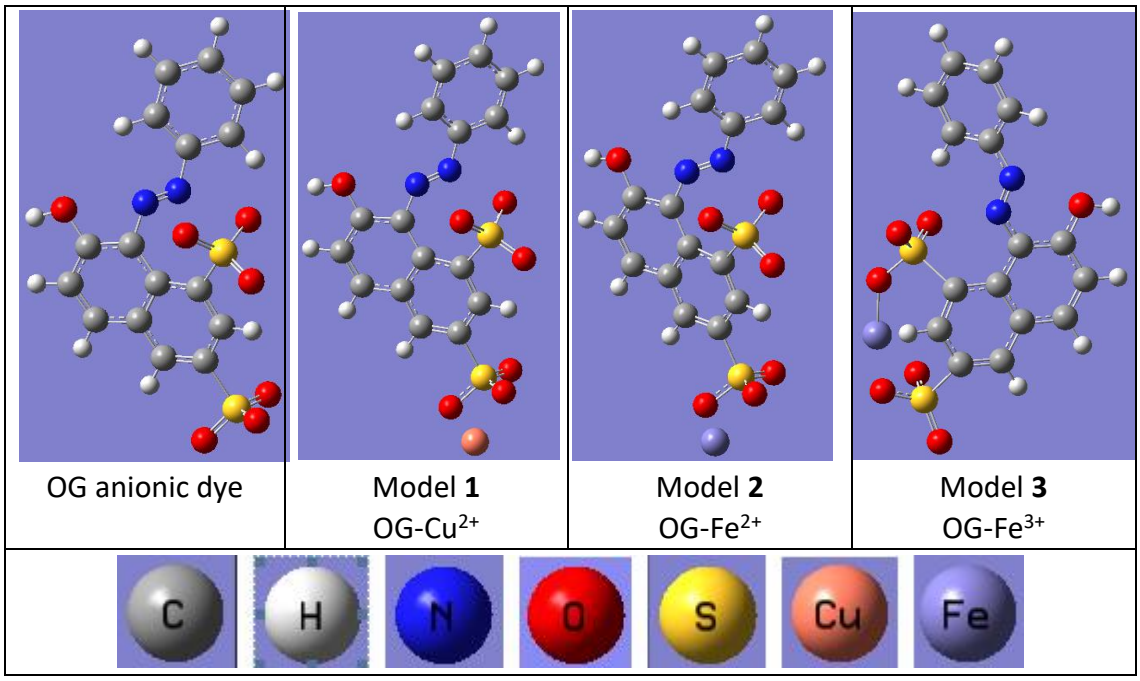

Fig. S2 The optimized structures of OG anionic dye and models **1-3** at B3LYP/6-31G(d) level by DFT.