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Electronic Supplementary Information

Iron Nanoparticles Decorated Boron Nitride Quantum Dots (Fe@BNQDs) as Improvement in Photo-Fenton Catalysis, Theoretical and Experimental Investigations

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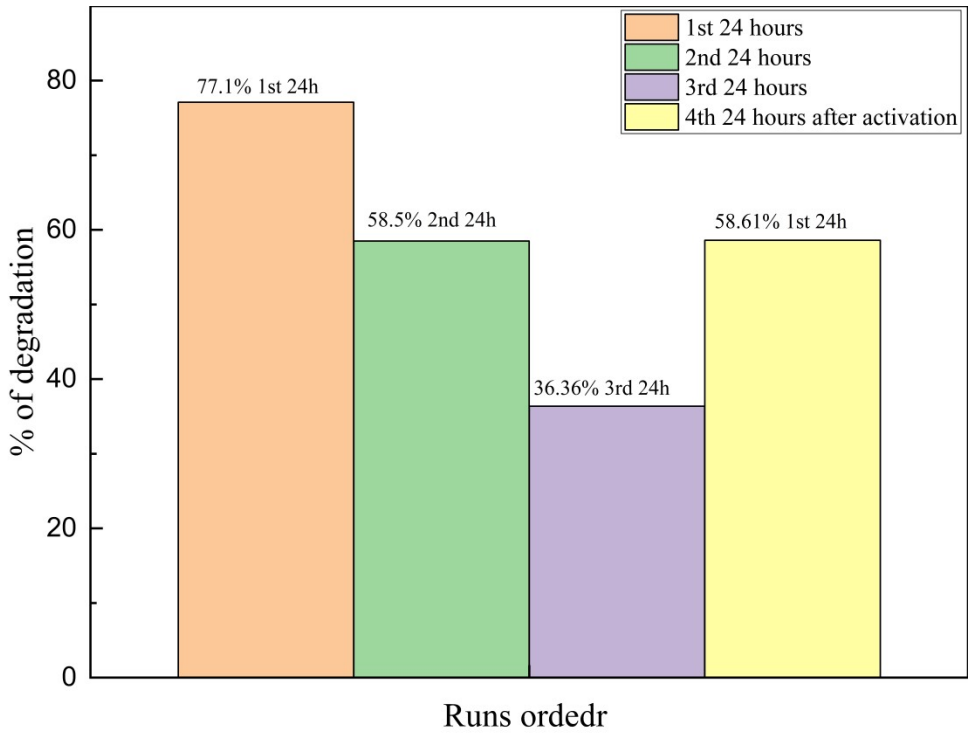

Figure S1. efficiency (time course) of photo-catalytic degradation of folic acid by Fe@BNQDs.

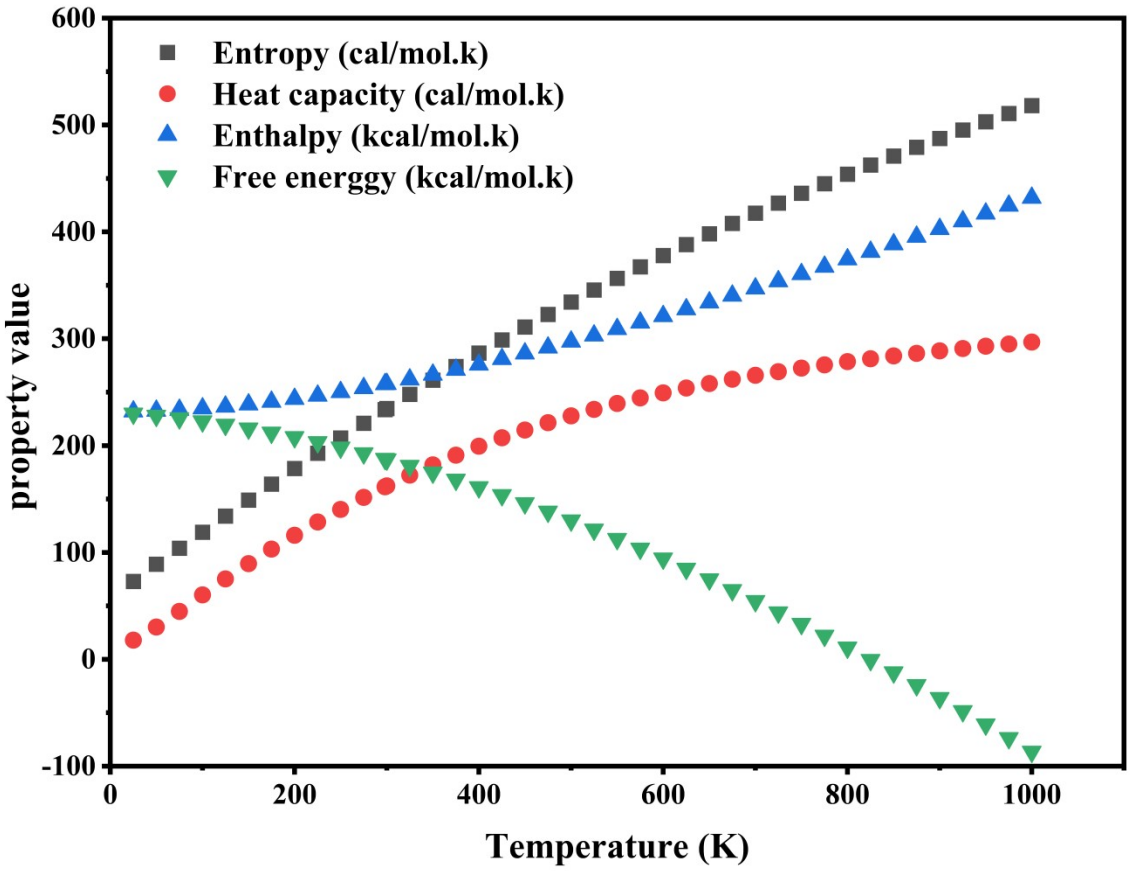

Figure S2. Thermochemical properties of Fe@BNQDs calculated for a single sheet by DFT/GGA/PBE Dmol[3] code.

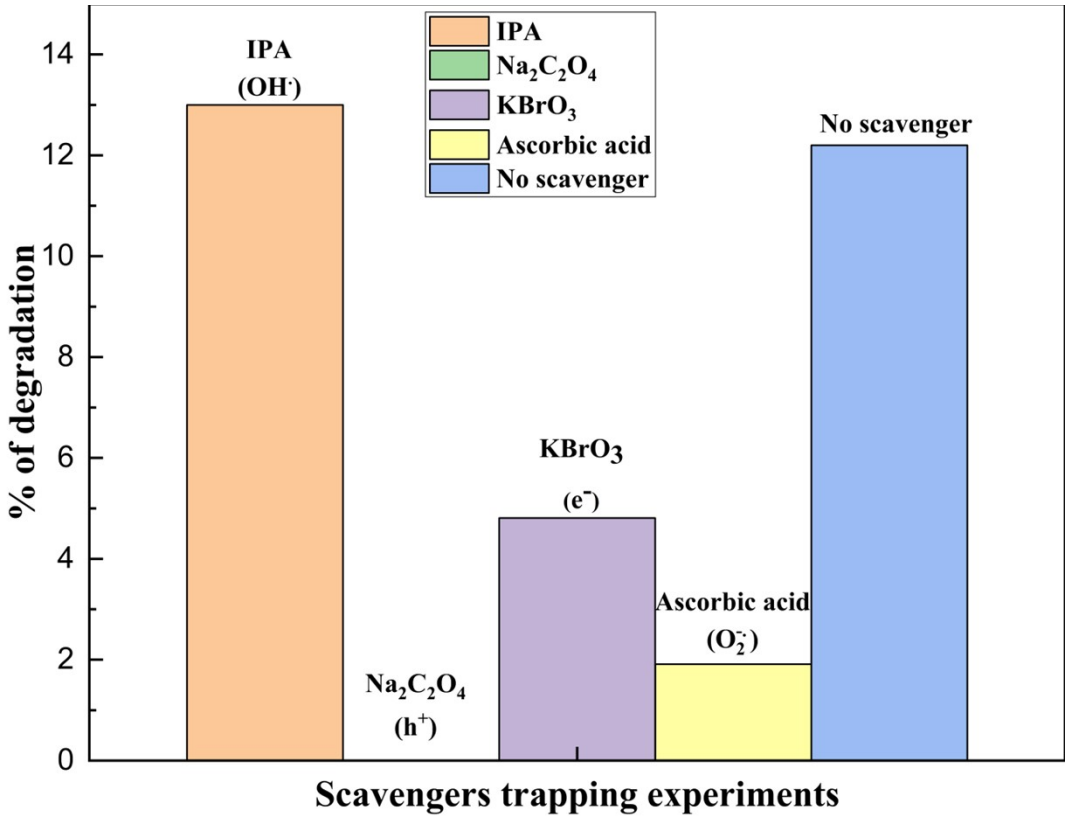

Figure S3. Scavengers trapping experiments of active species involved in photo-degradation of folic acid over Fe@BNQDs

Table S1. Analysis of Variance and estimated regression coefficient for percent of degradation of folic acid.

Source	DF	Coef.	Seq SS	Adj SS	Adj MS	F-value	P-value
Regression	9		187.126	187.126	20.7918	7.10	0.013
Linear	3		127.679	55.864	18.6213	6.36	0.027
Fe@BNQDs (g/mL)	1	192.879	57.453	25.114	25.1138	8.57	0.026
H2O2 (M)	1	56.306	37.563	34.762	34.7620	11.87	0.014
Temp.(C)	1	0.154	32.663	0.241	0.2411	0.08	0.784
Square	3		19.760	19.760	6.5866	2.25	0.183
Fe@BNQDs	1	-798.58	13.414	15.152	15.1518	5.17	0.063

(g/mL)*Fe@BNQDs (g/mL)							
H_2O_2 (M)*H_2O_2 (M)	1	-31.74	6.326	6.308	6.3079	2.15	0.193
	1	0.001	0.019	0.019	0.0193	0.01	0.938
Temp.(C)*Temp.(C) Interaction	3		39.688	39.688	13.2292	4.52	0.055
Fe@BNQDs (g/mL)*H2O2 (M)	1	115.25	5.313	5.313	5.3130	1.81	0.227
Fe@BNQDs (g/mL)*Temp.(C)	1	-2.825	7.981	7.981	7.9806	2.72	0.150
H2O2 (M)*Temp.(C)	1	-1.284	26.394	26.394	26.3939	9.01	0.024
Residual Error	6		17.578	17.578	2.9297		
Lack-of-Fit	4		16.569	16.569	4.1424	8.21	0.111
Pure Error	2		1.009	1.009	0.5043		
Total	15		204.704			R^2=91.41	

Table S2. the Calculated lattice parameters of Fe@BNQDs and h-BN.

	Lattice parameter (primitive cube)							**Bond length (Å)**	
Photo-catalyst	a(Å)	b(Å)	c(Å)	V(Å ^{3})	Alpha (α)	Beta (β)	Gamma (γ)	B-N	1.63
Fe@BNQDs	3.86947	3.86947	3.86947	57.936	90^o	90^o	90^o	B-Fe	1.82
								N-Fe	2.73
	Lattice parameter (Face cantered cubic)							**Bond length (Å)**	
h-BN	3.615	3.615	3.615	48.077	90^o	90^o	90^o	B-N	1.574

Table S3. The bandgap (Eg, eV) values of Fe@BNQDs nanostructure utilizing norm conserving pseudopotentials.

DMol3 code					
m-GGA/eV		GGA/eV		LDA/eV	
M06-L	0.868	BLYP Gremme & TS	1.072	PWC	0.762
M11-L	0.286	BOP	1.022	VWN	0.763
MS0	0.500	BP	0.904		
MS1	0.495	HCTH	1.019		
MS2	0.564	PBE	0.877		
Rev-TPSS	0.92	PBEsol	0.772		
TPSS	0.885	PW91	0.903		
		RPBE	0.899		
		VWN-BP	0.906		
CASTEP code					
Hybrid functions/eV		GGA/eV		LDA/eV	
B3LYP	Direct 1.839 **Indirect 2.295**	PBE	0.465	CA-PZ	0.626
HSE06	1.002	PBEsol	0.483		
		PW91	0.59		
		WC	0.503		
		RPBE	0.605		
Experimental value/eV				**2.39**	

Band Edges calculations

Band Edges (ECB, EVB) for Fe@ BNQDs ($Fe_{1.5}$ BNO_5=according to EDX results)

CB and VB for Fe@ BNQDs

$E_{VB} = X - E_c + 0.5E_g$

$E_{CB} = X - E_c - 0.5E_g$

$E_{VB} = E_{CB} + E_g$

$X = 1/2(E_{EA} + E_{IE})$

$$1eV = 1.6\times10^{-19}\,j = 1.6\times10^{-22}\,Kj$$

$$?\,\frac{Kj}{mol} = 1eV \times \frac{1.6\times10^{-22}\,Kj}{1eV} \times \frac{6.022\times10^{23}}{1mol} = 96.48\,\frac{Kj}{mol}$$

Calculations of X for Fe@ BNQDs:

B

- **E_{IE} = 800 kj/mol ÷ 96.48 = 8.29 eV**
- **E_{EA} = 27 kj/mol ÷ 96.48 = 0.2798 eV**

X_B = 1/2(8.29+0.2798) = 4.28 eV

O

- **E_{IE} = 1313.9 kj/mol ÷ 96.48 = 13.62 eV**
- **E_{EA} = 141 kj/mol ÷ 96.48 = 1.46 eV**

X_O = 1/2(13.62+1.46) = 7.54 eV

X_N = 7.3 eV

X_{Fe}= 4.0275 eV

This calculation are based on EDX results

Element	Wt.%
B	5.69
N	6.46
O	52.14
Fe	35.70

$\mathbf{X_{Fe@\ BNQDs} = (6124212.595)^{0.105} = 5.16\ eV}$

$E_{VB} = 5.16\ - 4.5 + (0.5 * 2.39\ eV) = 1.855\ eV$

$E_{CB} = 5.16\ - 4.5 - (0.5 * 2.39\ eV) = - 0.535\ eV$