Piezo-responsive bismuth ferrite nanoparticles mediated catalytic degradation of rhodamine-B and pathogenic *E. coli* in aqueous medium and its extraction using external magnetic stimulation after successful treatment

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Supporting information

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S1. DFT optimized structure of the BFO nanoparticle

Bi	0	0	0	0.000000000000	0.00000000	0.00000000
Bi	1	0	0	3.529691456332	0.00000000	0.00000000
Bi	2	1	0	3.712706735644	89.71821833	0.00000000
Bi	3	2	1	3.532825550519	90.35136264	0.00000000
Bi	1	2	3	3.481037717722	90.05628637	254.95622765
Bi	2	1	3	3.464317233366	89.93792212	105.04791976
Bi	3	2	1	3.532814720092	74.63259388	89.90320707
Bi	4	3	2	3.532842785039	89.97982471	74.67263468
Bi	8	4	3	2.805859683395	61.13961255	315.56806094
Fe	5	1	2	1.525308439300	42.56954489	39.89214362
Fe	3	2	1	1.184897300191	49.41744615	56.23991164
O	10	5	1	1.350878106492	84.11034855	314.85167642
H	12	10	5	0.970002244791	109.47153372	4.28763252
O	5	1	2	1.047186723799	116.97868084	57.46083258
H	14	5	1	0.970005015142	149.04284660	74.83211156
O	12	10	5	1.290795516997	67.16398733	239.40091005
H	16	12	10	0.969994026889	85.88793839	244.10514473
O	13	12	10	1.155832700437	114.46651324	48.43504325
H	18	13	12	0.970001483762	172.24233091	336.88212153
O	10	5	1	1.013848603787	141.69578084	107.36508146
H	9	8	4	0.828764996968	66.80225552	174.38064245
O	20	10	5	1.137041664012	75.60672717	202.68383176
H	17	16	12	0.730458381908	108.60677450	26.87772051
O	11	3	2	1.577885689934	89.42113582	102.97611269
H	24	11	3	0.970001913142	109.47109598	282.70068262
O	3	2	1	1.191871086360	78.46809399	311.16307991
H	26	3	2	0.969995399474	151.80327534	62.55519248

O	7	3	2	1.102180049085	35.25882077	342.37933383
H	28	7	3	0.969998541184	91.76191533	213.85713315
O	3	2	1	1.117259820812	109.47740740	163.74715188
H	30	3	2	0.969998355308	76.68937500	116.79235976
O	29	28	7	0.891583517849	64.82548798	151.06915070
H	9	8	4	0.264656832332	65.61119137	33.50149178
O	11	3	2	1.425160026137	112.43805097	280.87703221
H	27	26	3	0.710782867056	104.93900473	349.01702931

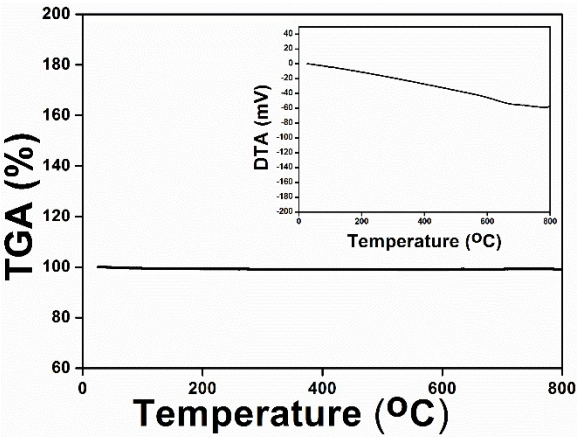

Fig. S1 TGA and DTA (inset) thermograms of BFO nanoparticles showing the thermal stability of the material