Electronic Supporting information

Nanocrystalline Ni-Zn spinel ferrites: size-dependent physical, photocatalytic and antioxidant properties

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Synthesis method

For synthesizing nickel-zinc ferrite nanoparticles, the chemical reagents $Ni(NO_3)_2.6H_2O$, $Fe(NO_3)_3.9H_2O$ and $ZnCl_2$ of analytical grade were used. All the raw chemicals were dissolved in a stoichiometric ratio in 200 ml of distilled water. The mixture was contained in a beaker and stirred constantly with a rotation of 800 rpm with the help of a magnetic stirrer. The precursor solution of sodium hydroxide was placed into the mixture drop by drop until the pH of the mixture reached 11 to produce precipitation. After that, the entire solution was heated at a constant temperature of 80 ^{0}C for 120 minutes to ensure that no elements were left un-reacted. Further, the solution was cooled down and washed several times using both distilled water and alcohol to get final pH of 7. The obtained precipitate was then dried out in an exposed atmosphere and ground to get fine a powder. After that, the powder sample was divided into three equal parts and sintered at three different temperatures 400 ^{0}C, 600 ^{0}C and

800 ^{0}C respectively for 5 hours in a muffle furnace to obtain size variation.[19] During calcination, the temperature of the furnace was raised at a constant rate and then steadily cooled down to escape the quenching effect. Dark-brown powder samples of Ni-Zn ferrite nanoparticles were collected and indexed as ZNF-1, ZNF-2 and ZNF-3 based on increasing average size. All the physical characterizations were performed with these obtained samples.

Characterization techniques

X-ray diffractograms (XRD) were recorded at 300 K using Bruker D8 Advance powder X-ray diffractometer with Cu-K$_\alpha$ source having wavelength 1.5406 Å. Powder samples were scanned within the angular range of 20^0 to 80^0 at a scan rate of 0.05^o/sec and data was collected. The x-ray diffractometer was operated at a voltage of 40 kV and a current of 40 mA respectively. The average particle size, shape and morphology of synthesized nanoparticles were examined with the help of HRTEM (JEM-2100F, JEOL, Japan) with an accelerating voltage of 200 kV. Surface morphology of the nanocatalysts were investigated using FESEM microscopy (FESEM, JEOL-JSM 5600) along with EDS at room temperature. Room temperature FTIR spectra of as-prepared nanoparticles were collected using the Perkin-Elmer FTIR spectrophotometer. All the magnetic measurements were performed using 16 T-VSM-PPMS (Quantum design). Investigation of surface charge and zeta potential of ferrite nanoparticles was performed at room temperature using a zeta potential analyzer (Malvern-NanoZS90). The specific surface area of all the nanocatalysts was obtained from N$_2$ adsorption–desorption isotherms by employing Brunauer–Emmett–Teller (BET) method (Quantachrome iQ autosorb analyzer, USA) and the mean pore size was measured with the help of Barrett–Joyner–Halenda (BJH) approach. UV DRS spectrometer (UV-2550, Shimadzu, USA) was utilized in collecting the absorption data, methylene blue (MB) dye-degradation data and antioxidant properties of entire ferrite samples.

Sample Id	ZNF-1	ZNF-2	ZNF-3
Unit cell parameters			
Space group	Fd-3m	Fd-3m	Fd-3m
$a = b = c$ (Å)	8.371	8.376	8.381
$\alpha = \beta = \gamma$ (degree)	90	90	90
Volume (Å^3)	586.58	587.64	588.69
D (nm)	16.4	21.1	38.3
Microstrain (X 10^{-4})	9.74	11.63	5.71
ρ (g/cm^3)	5.348	5.351	5.354
u ($\pm$ 0.001)	0.378	0.378	0.378
L$_A$ (Å)	3.625	3.627	3.629
L$_B$ (Å)	2.959	2.961	2.963
Refinement parameters			
R_{wp}(%)	3.82	4.11	3.77
R_p(%)	3.05	3.26	3.02
χ^2	1.09	1.04	1.12

Table S1: Contains unit cell parameters and Rietveld refinement factors of all the Ni-Zn ferrite samples.

Sample Id	R^2 for 1st order kinetics	R^2 for 2nd order kinetics
ZNF-1	0.961	0.768
ZNF-2	0.973	0.889
ZNF-3	0.992	0.981

Table S2: Contains regression correlation coefficient (R^2) of kinetics model.
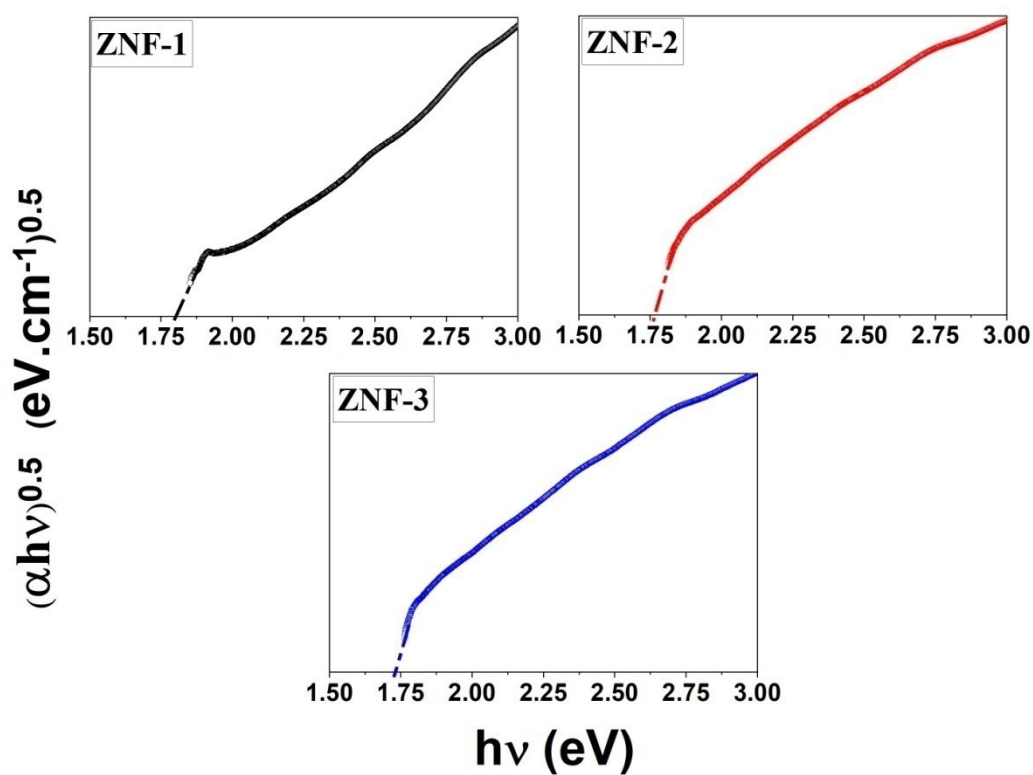
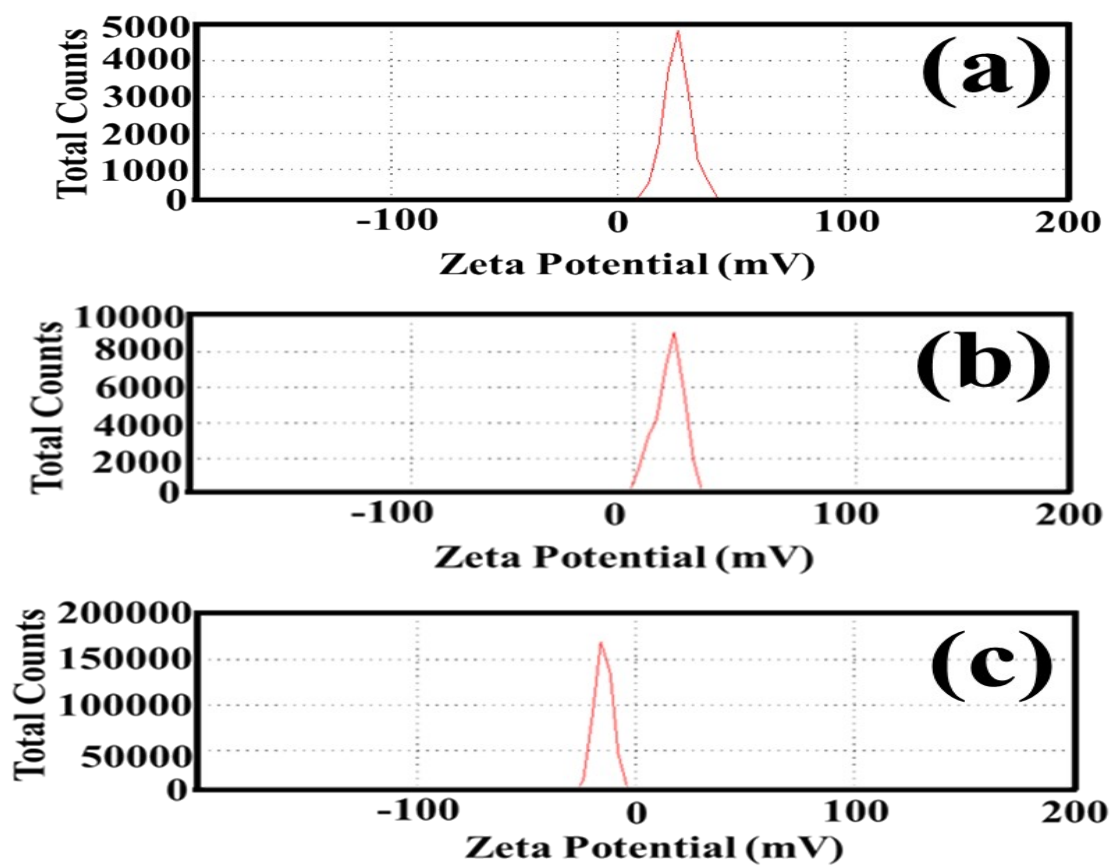Figure S1: Tauc plot for all the samples obtained at room temperature.

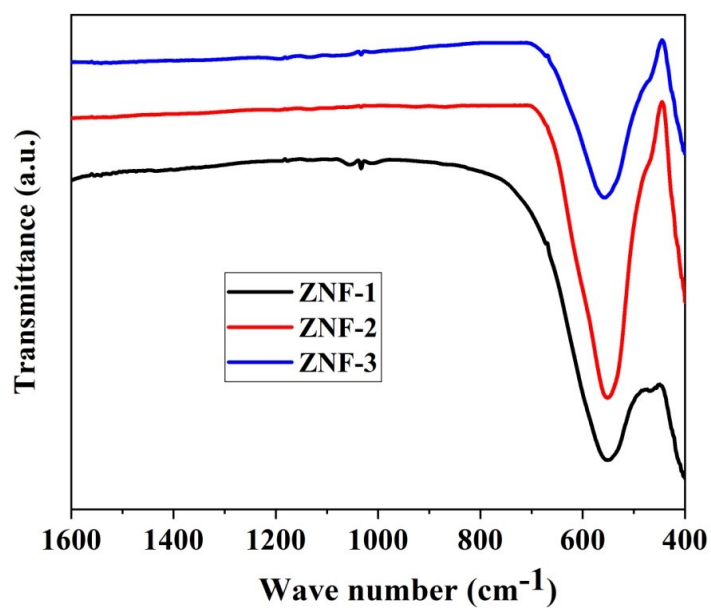Figure S2: (a-c) Zeta potential graphs of ZNF-1 ZNF-2 and ZNF-3 ferrite samples.

Figure S3: Room temperature FTIR spectra of Ni-Zn ferrite samples.
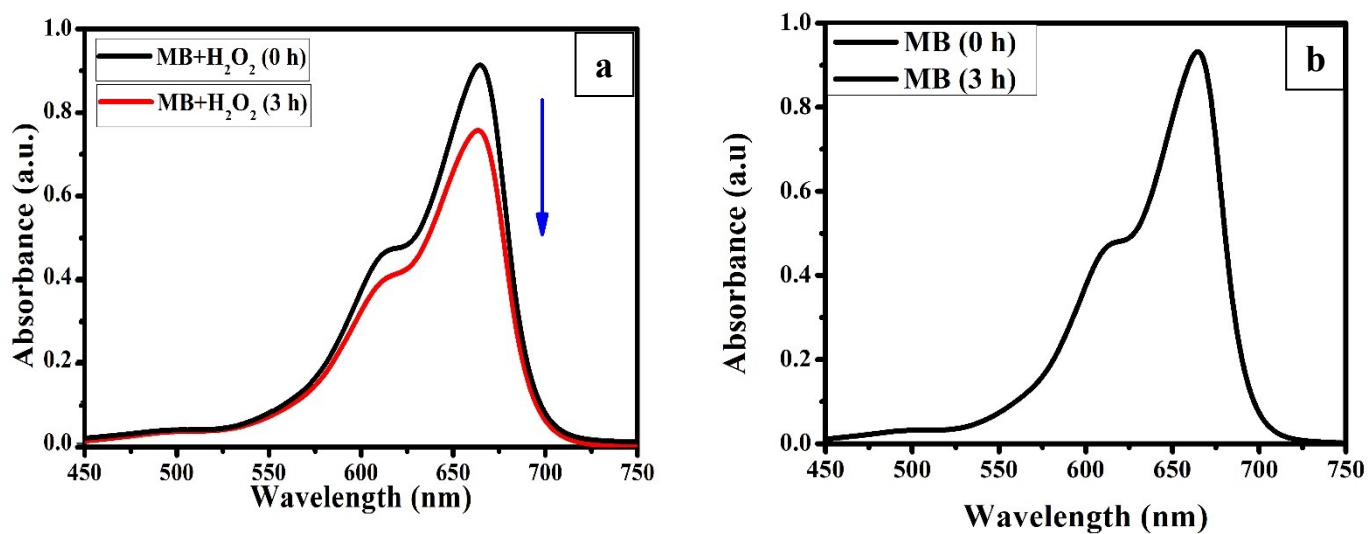
Figure S4: Photon mediated degradation of MB (a) with only H_2O_2 and (b) without catalyst

and H_2O_2
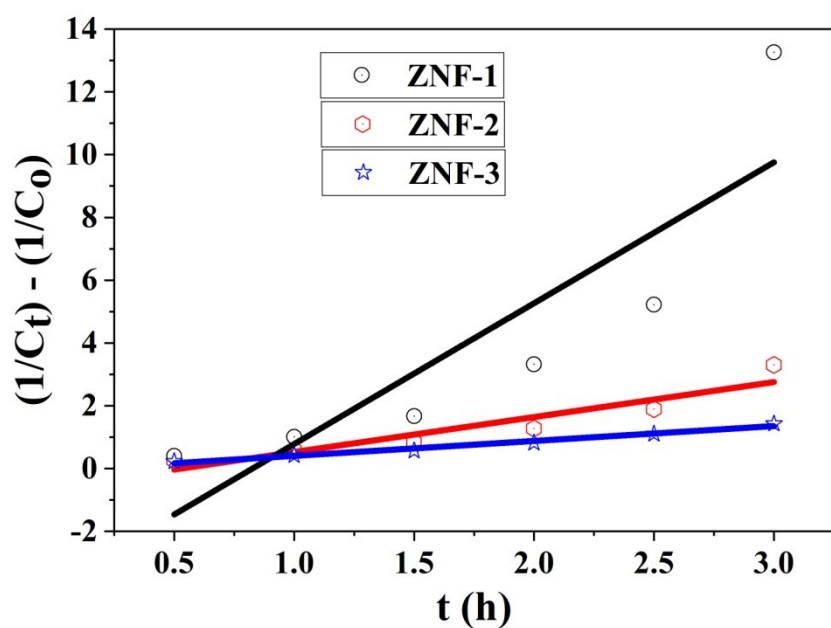
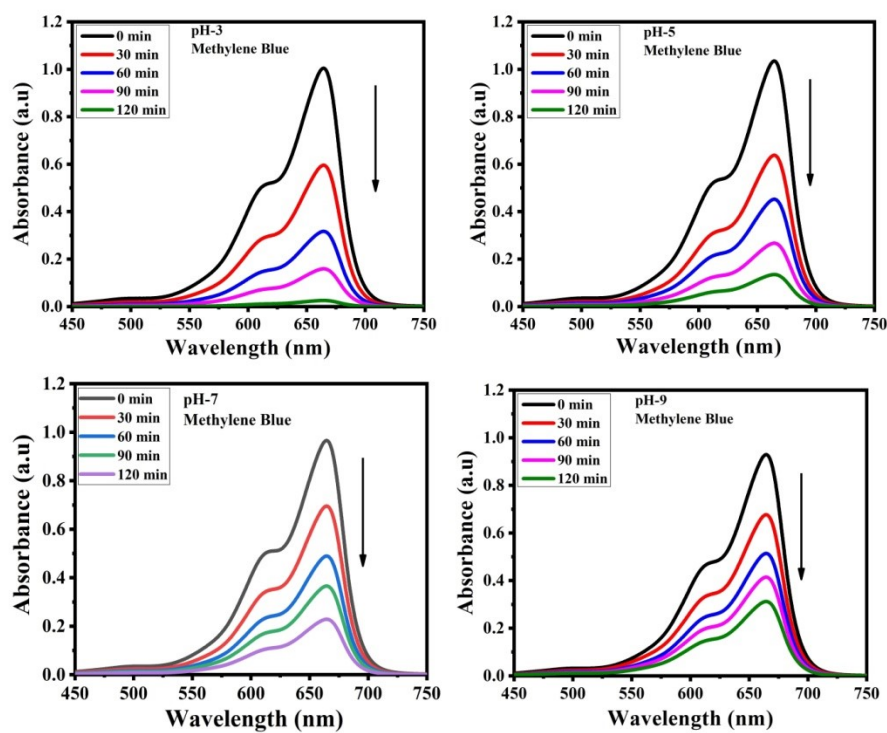Figure S5: Rate constant of 2nd order kinetics model

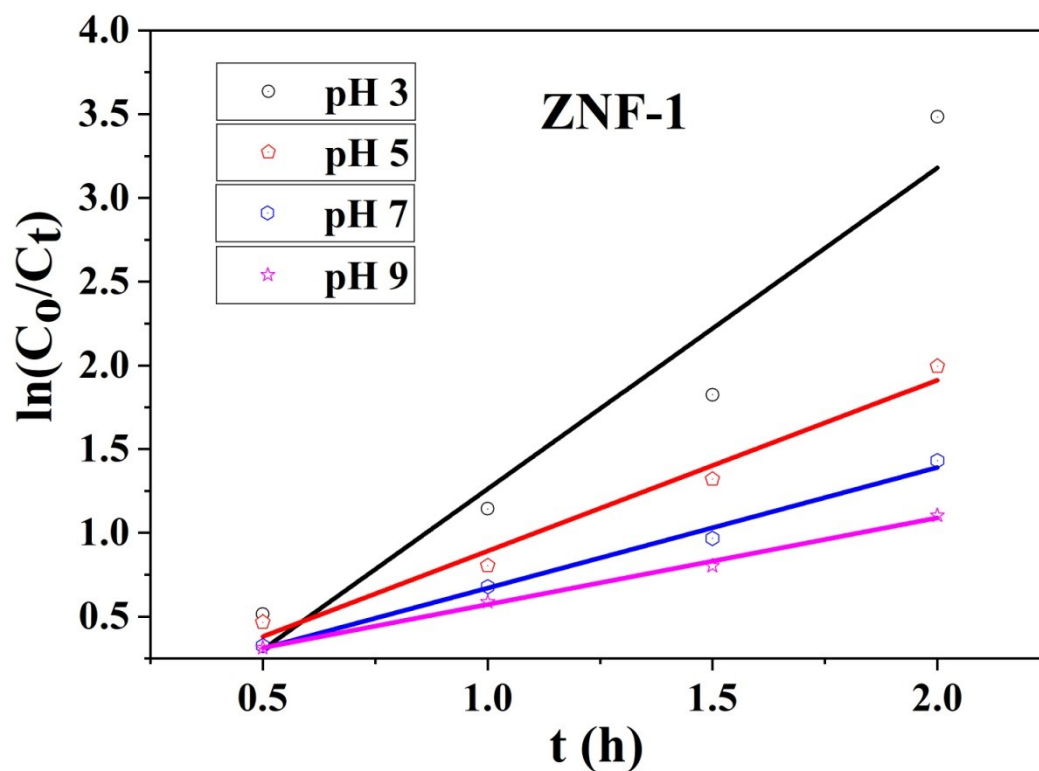Figure S6: Reduction of MB in different pH using ZNF-1 sample

Figure S7: Rate constant of ZNF-1 sample at different pH (1st order kinetics model)
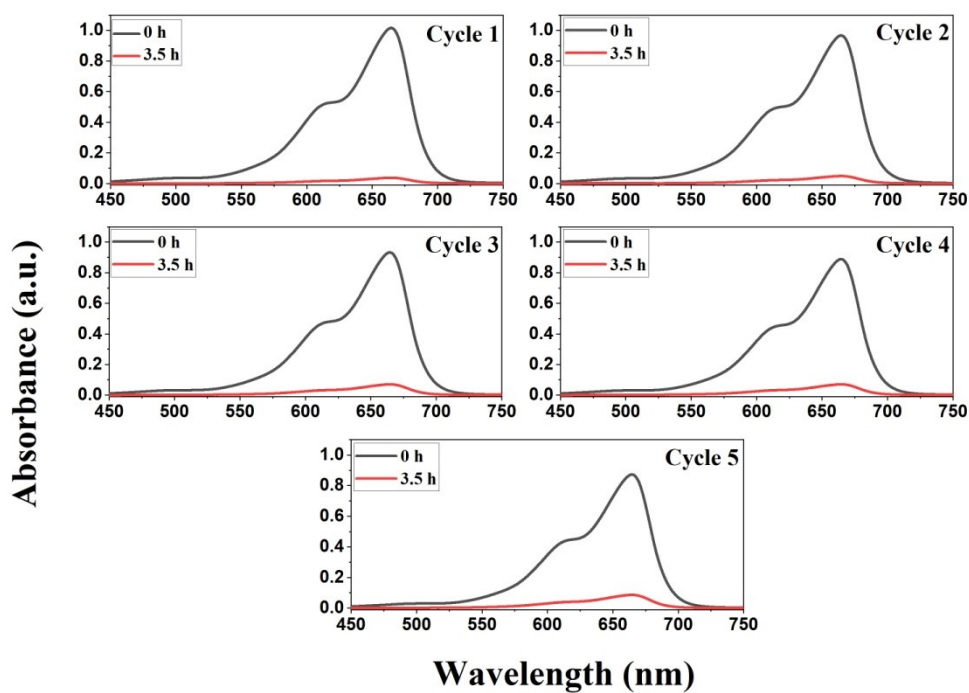

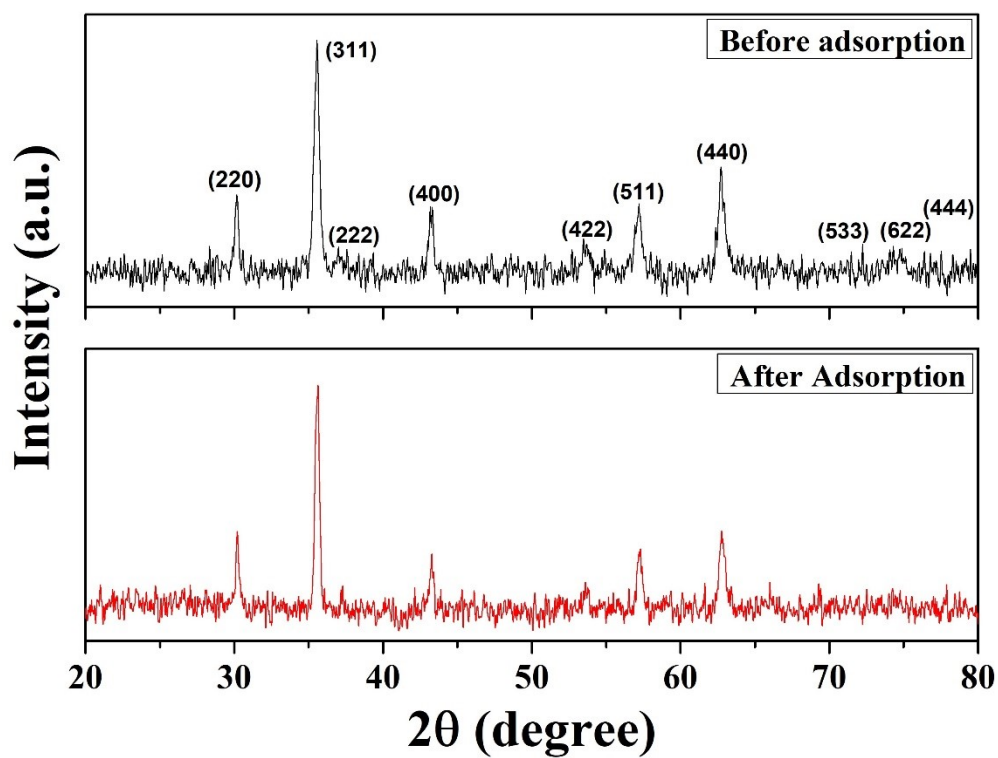Figure S8: Reusability of ZNF-1 sample (five cycles)
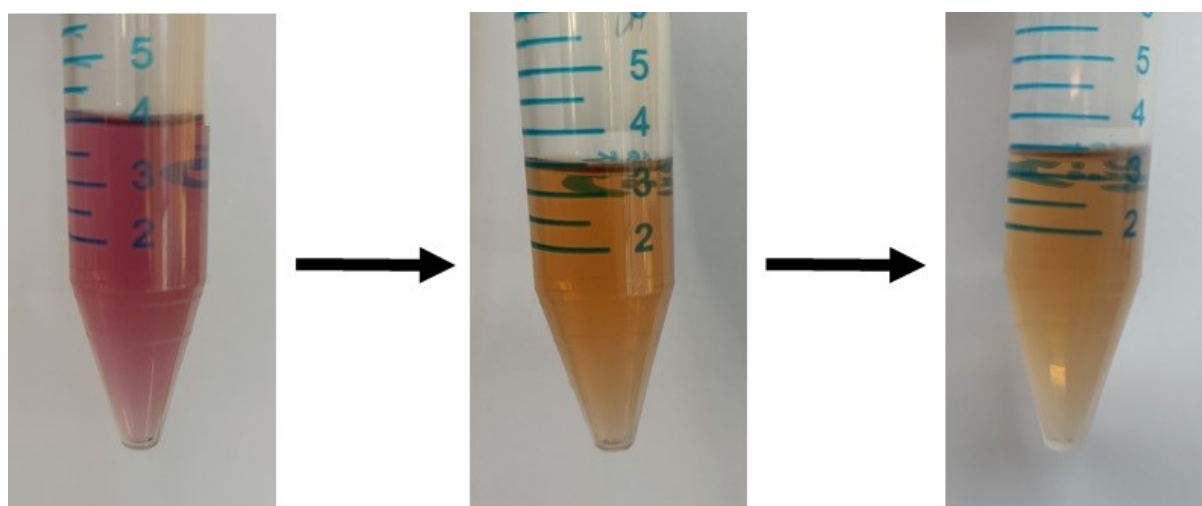
Figure S9: PXRD patterns of ZNF-1 sample recorded at RT before and after adsorption

Figure S10: Color change of DPPH solution