Supplemental materials for:

Photoelectrochemical Response and Electronic Structure Analysis of Mono-Dispersed Cuboid-Shaped Bi$_2$Fe$_4$O$_9$ with Strong Near-Infrared Absorption

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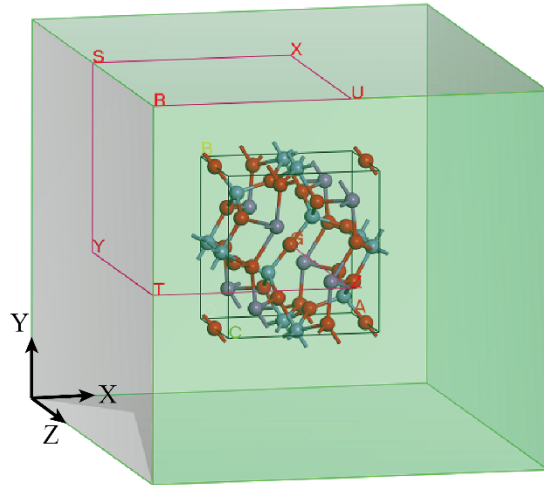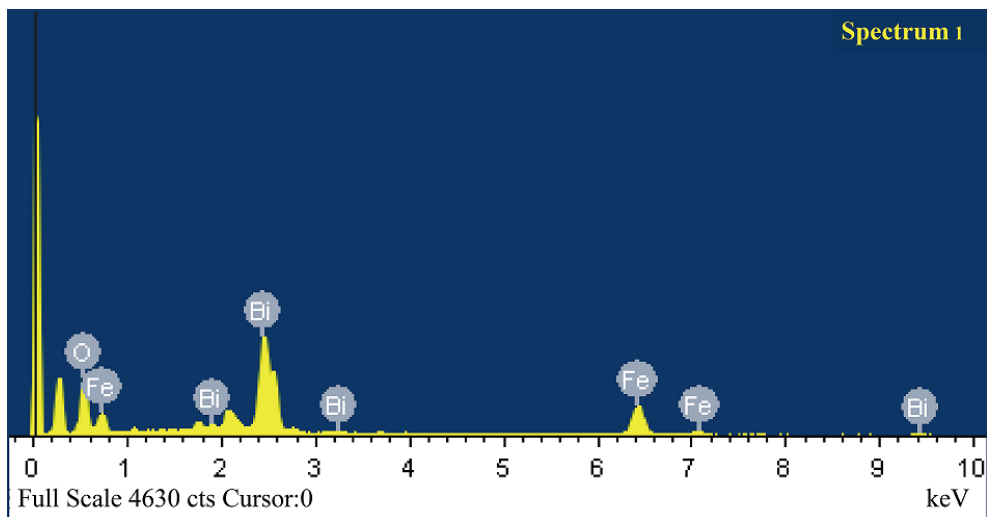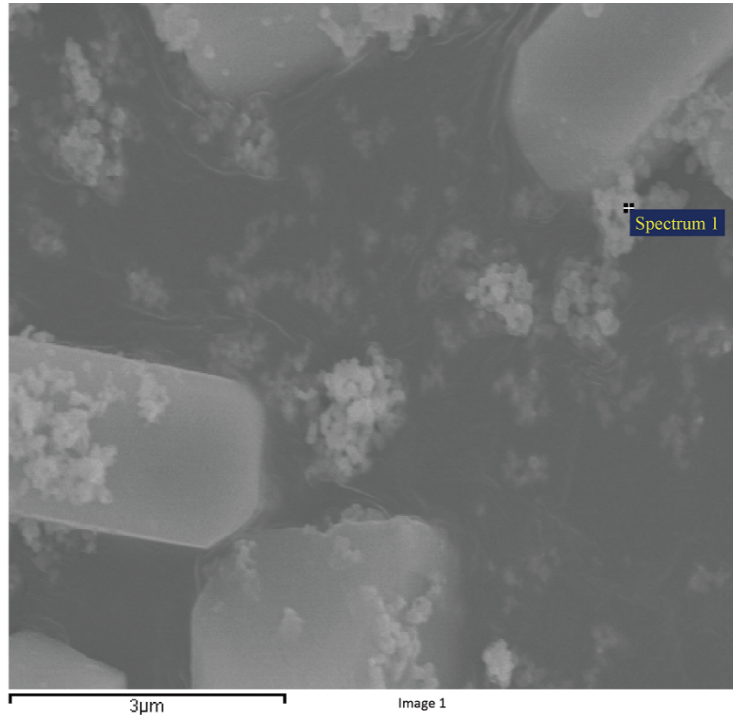Tel: +86-21-34202549

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Figure S1: The k-points sampling in Brillouin zone of the $Bi_2Fe_4O_9$ (BFO) conventional unit cell.

Elements	wt. %	at. %
O K	21.44	65.40
Fe K	25.38	22.18
Bi M	53.18	12.42
Total	100.00	

Figure S2: EDS data of the fragments around the BFO cuboids. The C and Pt peaks

that originate from the conductive tape and the Pt coating, correspondingly, for

enhancing conductivity are not shown. The ratio of Fe: Bi in the fragments is 1.78:1

which is similar to that in BFO cuboids.

Figure S3: The light brown transparent solution of $Fe(OH)_3$ (a) and its Tyndall effect (b).

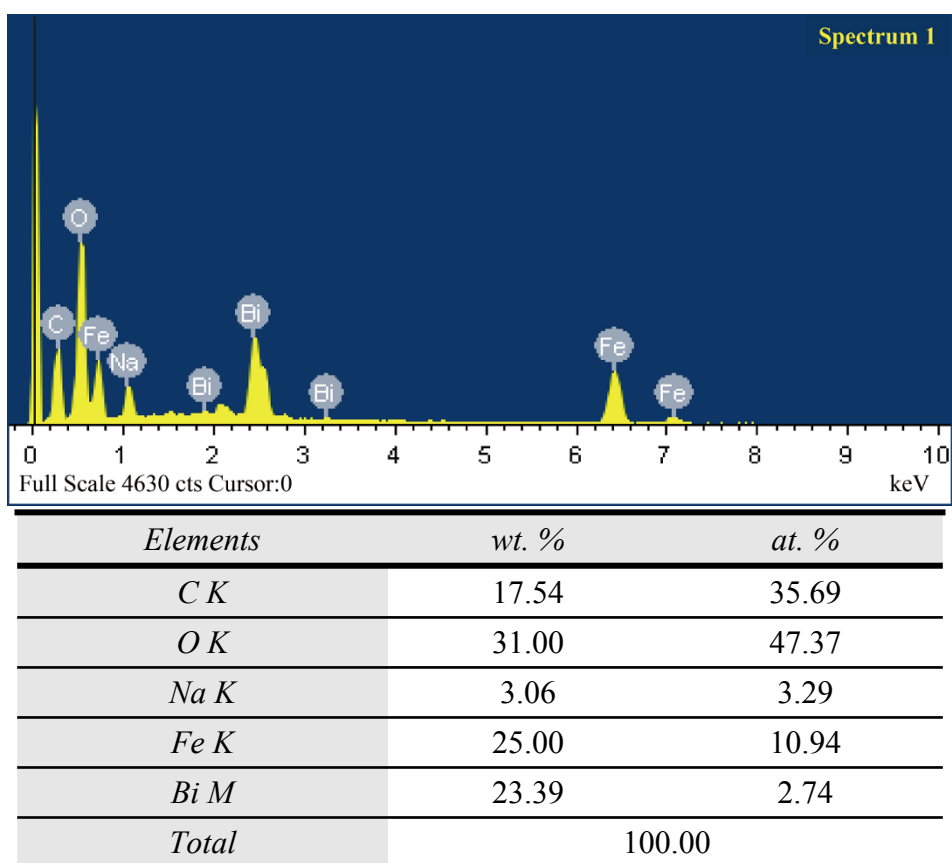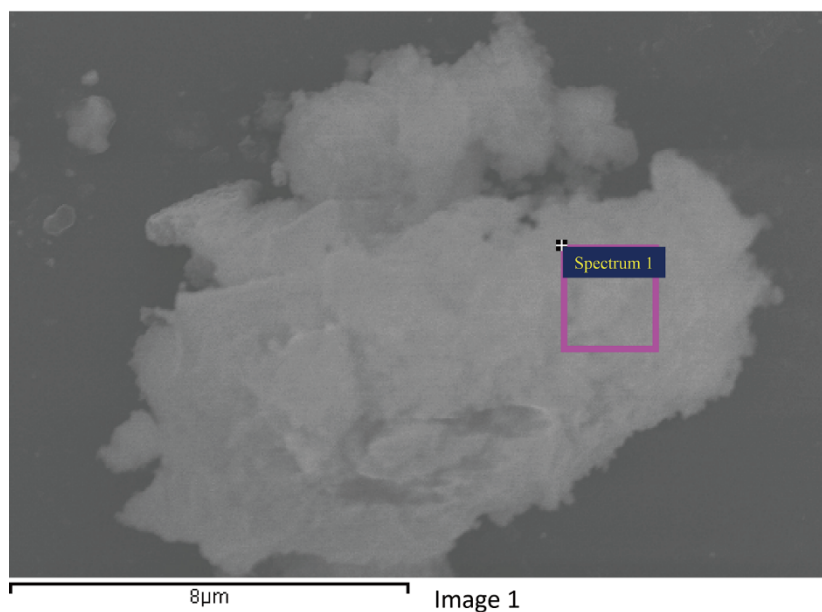| Elements	wt. %	at. %
C K	17.54	35.69
O K	31.00	47.37
Na K	3.06	3.29
Fe K	25.00	10.94
Bi M	23.39	2.74
Total	100.00	

Figure S4: EDS data of the dried sol. The C peak is originated from the conductive

tape. The brown sol is dried at 60 ℃ for 12h to remove all solvent. The content of Fe

in the dried sol is 4 times to that of Bi implying the brown sol is primarily composed

by iron hydroxide.

Interplanar spacing formula in orthorhombic system:

$$d = \frac{1}{\sqrt{\left(\dfrac{h}{a}\right)^2 + \left(\dfrac{k}{b}\right)^2 + \left(\dfrac{l}{c}\right)^2}}$$

Lattice parameters of $Bi_2Fe_4O_9$: a=0.794 nm, b=0.844 nm, c=0.601 nm

$d_{(141)}$= 0.1931 nm
$d_{(330)}$= 0.1928 nm

Fig S5: Calculation of the interplanar spacing of (141) plane and (330) plane. In many

papers, the peak at ~47° is usually indexed as (141). Based on the calculation above,

the diffraction peak of (330) will as well appear at ~47°, that's why this peak is also
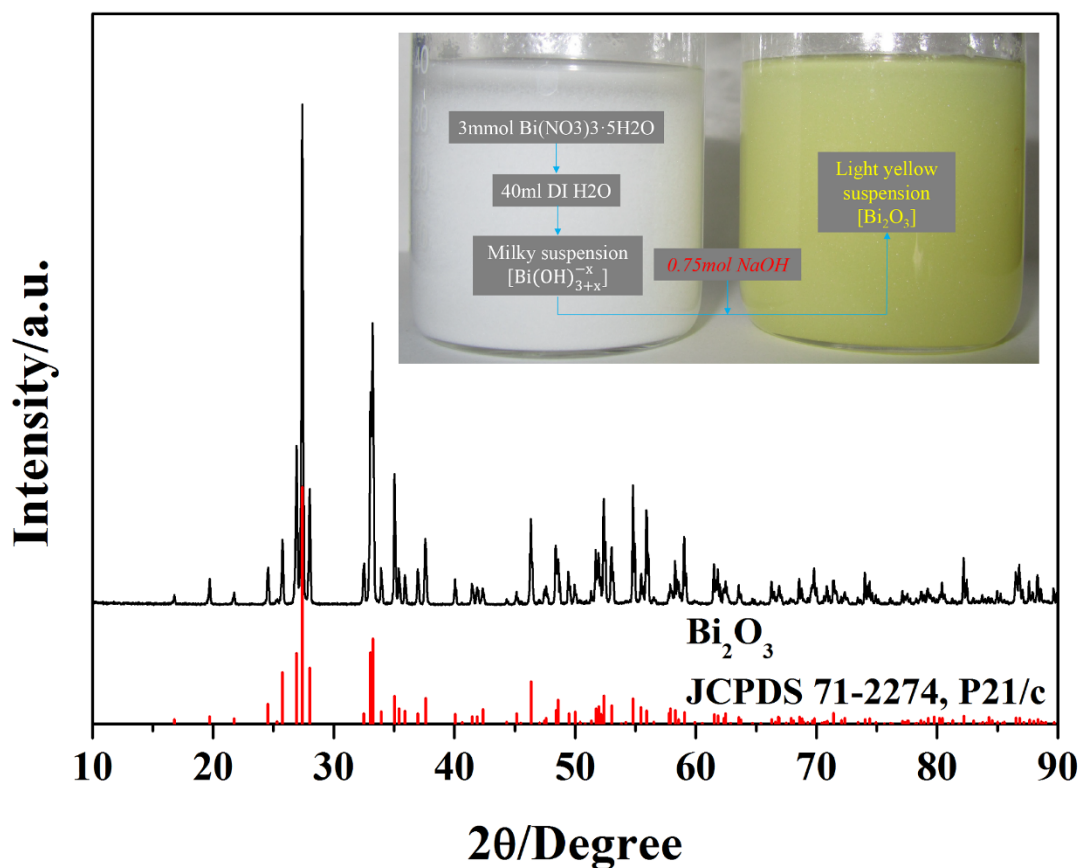
strengthened in the XRD pattern of DB-BFO.

Figure S6: The XRD pattern of the light yellow precipitate dried at 60 ℃, the standard XRD pattern of Bi_2O_3 with a space group of P21/c is listed below. The light yellow precipitate is obtained as follows. 0.3 mmol $Bi(NO_3)_3 \cdot 5H_2O$ was added into 40 ml DI water under constant stirring for 1 h and a homogeneous milky suspension was formed as described in the manuscript. The milk-white suspension turned into a light yellow suspension promptly upon the addition of 0.75 mol NaOH, as shown in the inset.
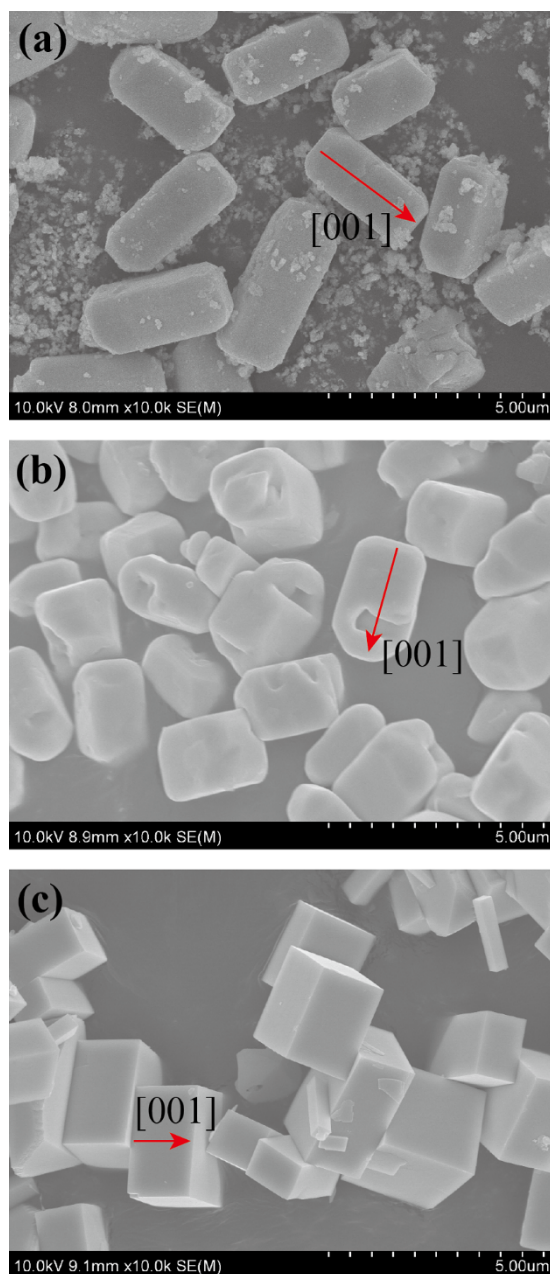
Figure S7: FE-SEM images of $Bi_2Fe_4O_9$ crystals synthesized at 180 ℃ with various concentrations of NaOH: (a) 18.75 M NaOH, (b) 12.5 M NaOH, and (c) 6.25 M NaOH for 24 h.
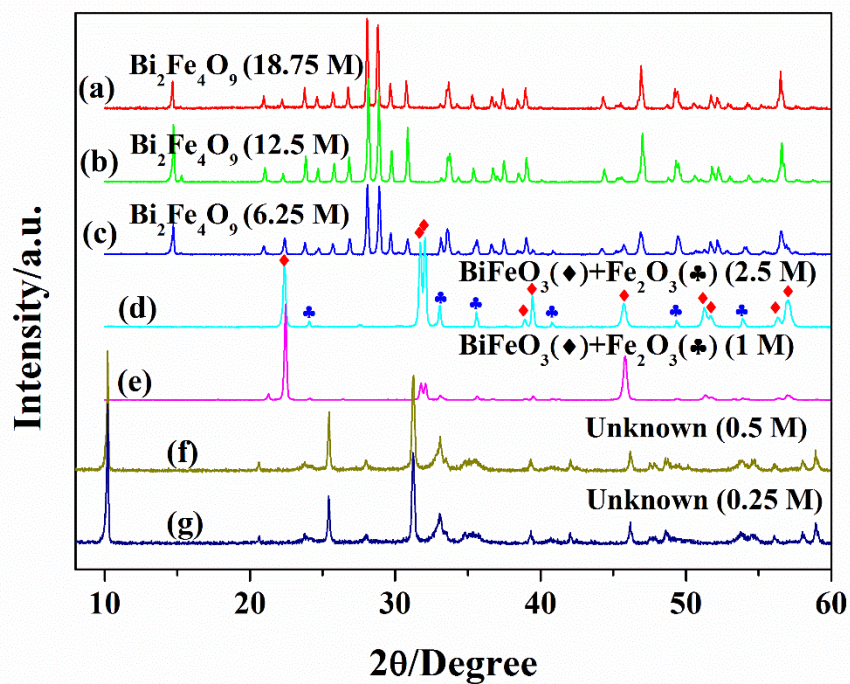
Figure S8: XRD patterns of the products synthesized in various concentrations of NaOH: (a) 18.75 M, (b) 12.5 M, (c) 6.25 M, (d) 2.5 M, (e) 1 M, (f) 0.5 M and (g) 0.25M at 180 ℃ for 24 h.
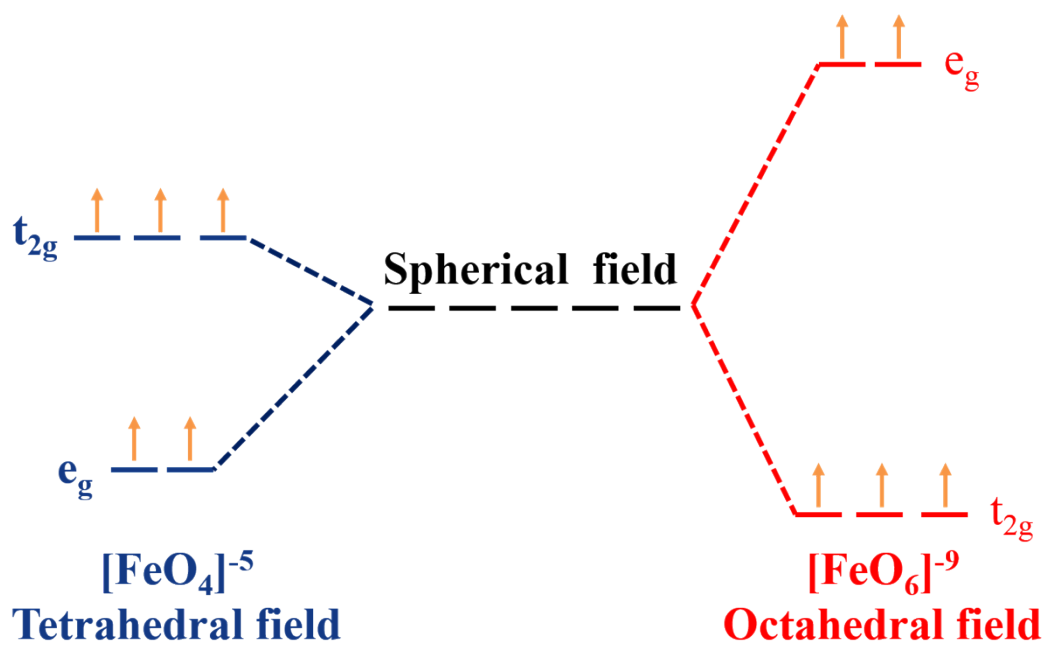
Fig S9: Schematic electronic DOS of Fe^{3+} in octahedral O_h and tetrahedral T_d coordination.