Electronic supplementary information

Optimizing the photocatalysis in ferromagnetic $Bi_6Fe_{1.9}Co_{0.1}Ti_3O_{18}$ nanocrystal by morphology controlling

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The calculation method of {117} facets:

We determined the {117} facets by the following method. The cell parameters of BFCTO-2.00 sample calculated from the refinement of the XRD pattern by using the Pawley method are a=5.680Å, b=5.407 Å and c=49.991 Å. From the SEM image and the laterally-viewed TEM image, the interfacial angle (θ) between the top parallel surface and the lateral surface was about 61.5° as shown in Fig. 2(c) and Fig. 3(c). Besides, the two top parallel surface could be indexed to (001) and $(00\bar{1})$ facets, respectively. According to the SAED image (the insert of Fig. 3(f) in the manuscript) and the formula of interfacial angle of orthorhombic lattice,[1] we listed the interfacial angle (θ) between the top parallel {001} facets and the lateral {hkl} facets in Table 1. The θ value of 61.23° is the nearest to 61.5°, therefore, the lateral surfaces were determinated to be {117}.

$$\cos\theta = \frac{\frac{h_1h_2}{a^2}+\frac{k_1k_2}{b^2}+\frac{l_1l_2}{c^2}}{\sqrt{\left(\frac{{h_1}^2}{a^2}+\frac{{k_1}^2}{b^2}+\frac{{l_1}^2}{c^2}\right)\left(\frac{{h_2}^2}{a^2}+\frac{{k_2}^2}{b^2}+\frac{{l_2}^2}{c^2}\right)}} = \frac{2l_2}{\sqrt{310{h_2}^2+340{k_2}^2+4{l_2}^2}}$$

Table 1 The interfacial angle (θ) between the top parallel {001} facets and the lateral {hkl} facets. (The 61.23° interfacial angle and corresponding facets are marked in green)

the lateral surface (hkl)	the interfacial angle (θ)
{111}	85.51 °
{113}	76.76 °
{115}	68.58 °
{117}	61.23 °
{119}	54.78 °
{11$\underline{1}$1}	49.21 °
{11$\underline{1}$3}	44.44 °
{11$\underline{1}$5}	40.36 °
{11$\underline{1}$7}	36.86 °
{11$\underline{1}$9}	33.86 °
{11$\underline{2}$1}	31.26 °
{11$\underline{2}$3}	29.00 °
{11$\underline{2}$5}	27.02 °
{11$\underline{2}$7}	25.27 °
{11$\underline{2}$9}	23.73 °

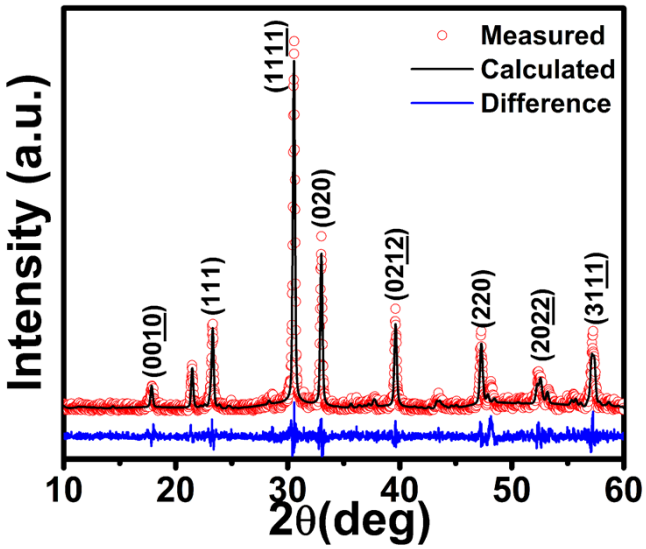

Fig. S1 The refinement XRD patterns of BFCTO-2.00. Red circles indicate the experimental data and the calculated data are the continuous black line overlapping them. The lowest blue curve shows the difference between the experimental and calculated patterns.

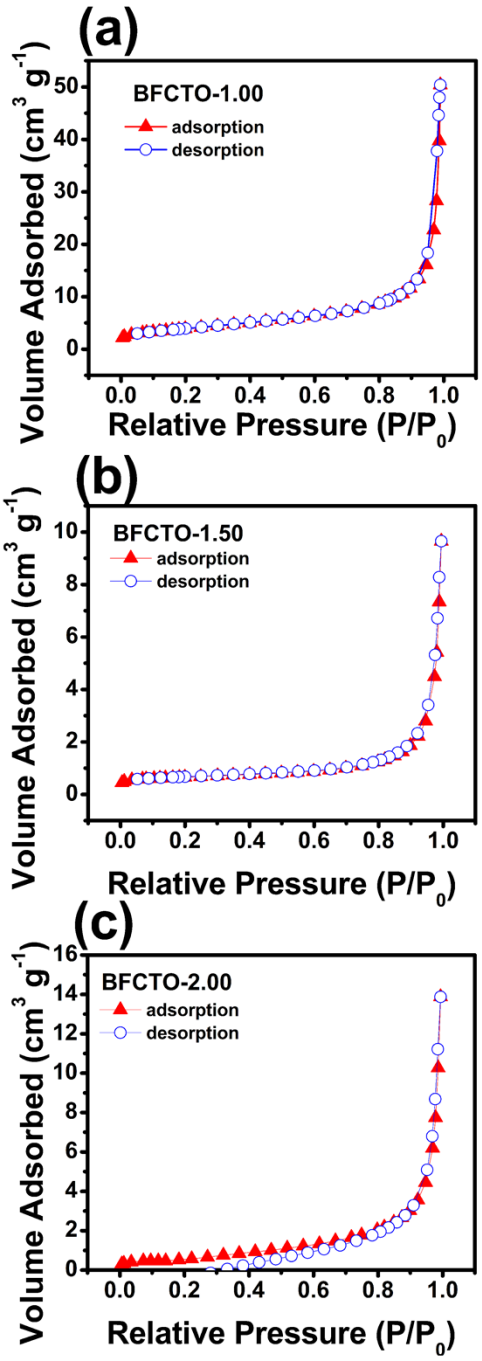

Fig. S2 Nitrogen adsorption–desorption isotherms of (a) BFCTO-1.00, (b) BFCTO-1.50 and (c) BFCTO-2.00.

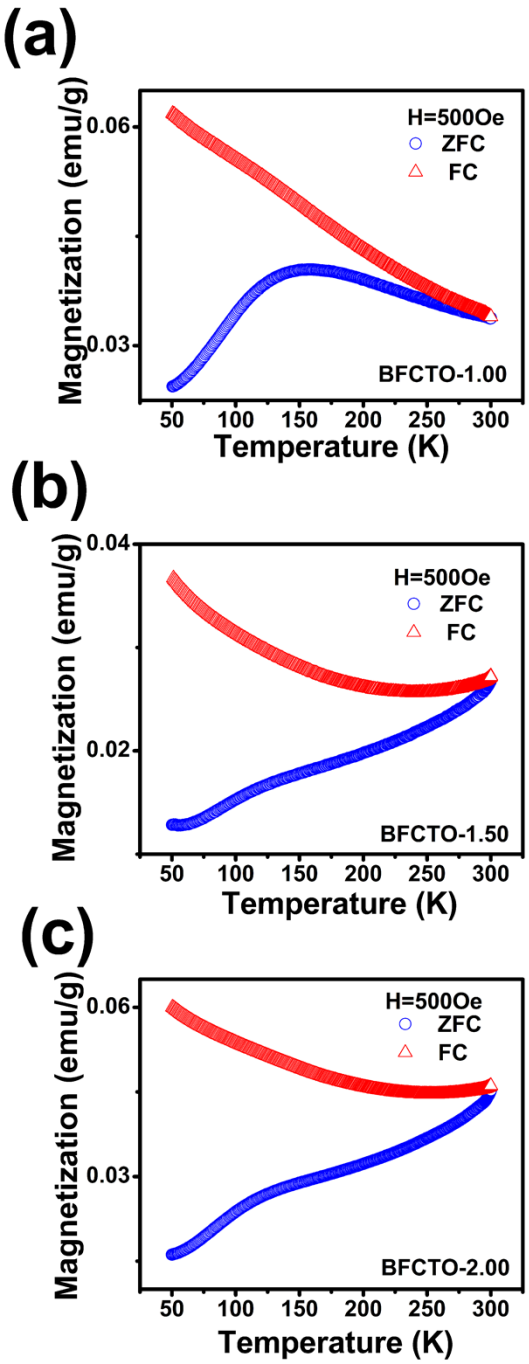

Fig. S3 Zero-field-cooled (ZFC) and field-cooled (FC) magnetization curves of (a) BFCTO-1.00, (b)BFCTO-1.50 and (c) BFCTO-2.00 under a magnetic field of 500Oe.

References:

1. R. J. D. Tilley, *Crystals and crystal structures*, John Wiley & Sons, Ltd., 2006, p. 37.