

## Supporting information

### Preparation and Characterization of the Possible Topological Insulator BiYO<sub>3</sub>, Experiment versus Theory

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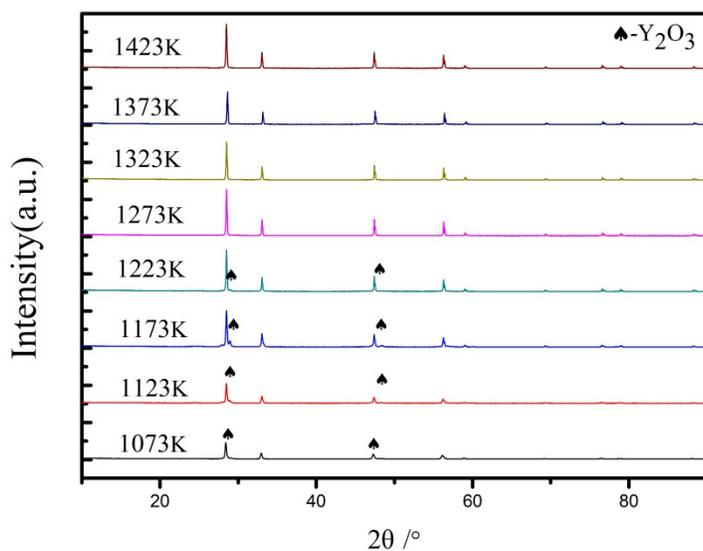
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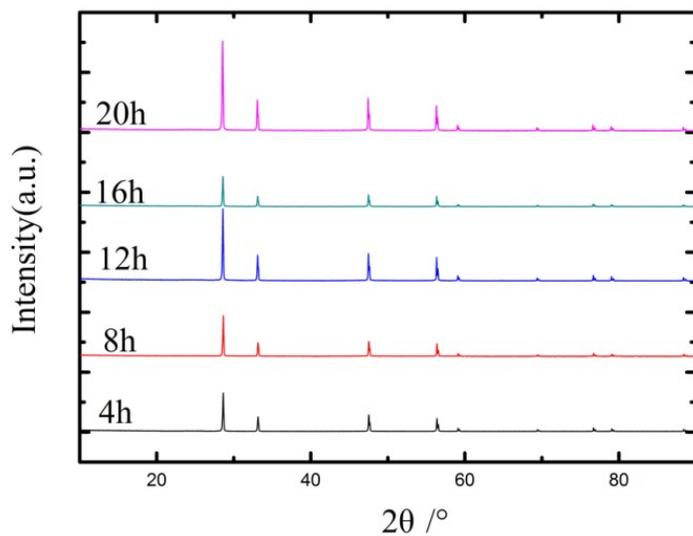
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#### X-ray powder diffraction of Bi-Y-O system.

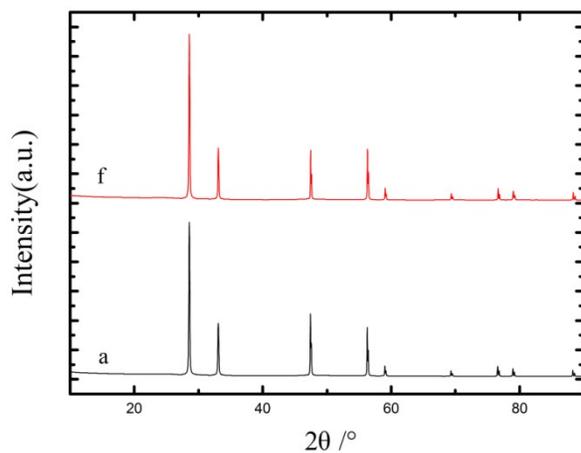
The system Bi-Y-O has been studied by X-ray powder diffraction, as shown in Figure S1-S4, for exploring the preparation process of BiYO<sub>3</sub>. The samples in Figure S1-S3 were all synthesized under ambient pressure with molar ratio of starting materials Bi<sub>2</sub>O<sub>3</sub>:Y<sub>2</sub>O<sub>3</sub>=1:1. In Figure S1, samples were sintered in the temperature range of 1073 to 1423 K with a step interval  $\Delta T = 50$  K for exploring the suitable reaction temperature. In Figure S2, samples were sintered for the reaction time between 4 and 20 hours in a step interval,  $\Delta t = 4$ h for exploring the suitable reaction time. In Figure S3, samples were cooled in the furnace or in the air. In Figure S4, 13 different starting ratios ranging from 20 to 60% mol of Y<sub>2</sub>O<sub>3</sub> have been used with the optimized conditions to study the phase diagram.



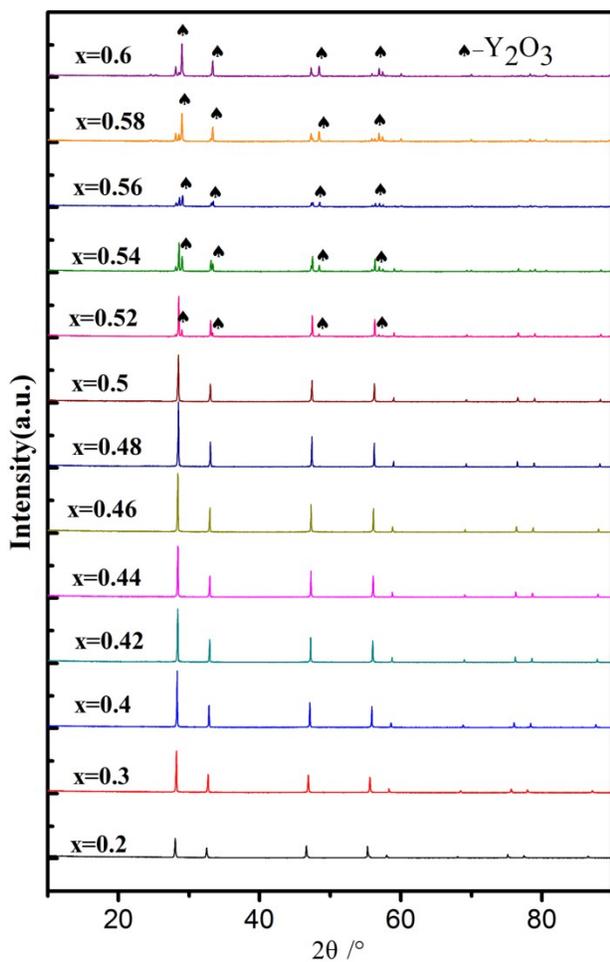
**Figure S1.** XRD patterns of samples which were sintered under the temperature (1073 to 1423 K,  $\Delta T = 50$  K) with 4 h of reaction time and cooled in the furnace.



**Figure S2.** XRD patterns of samples which were sintered under 1273 K with reaction time (4 h-20 h,  $\Delta t=4$  h) and cooled in the furnace.



**Figure S3.** XRD patterns of samples which were sintered under 1273 K with 20h of reaction time and cooled in the furnace (f) or the air (a), respectively.



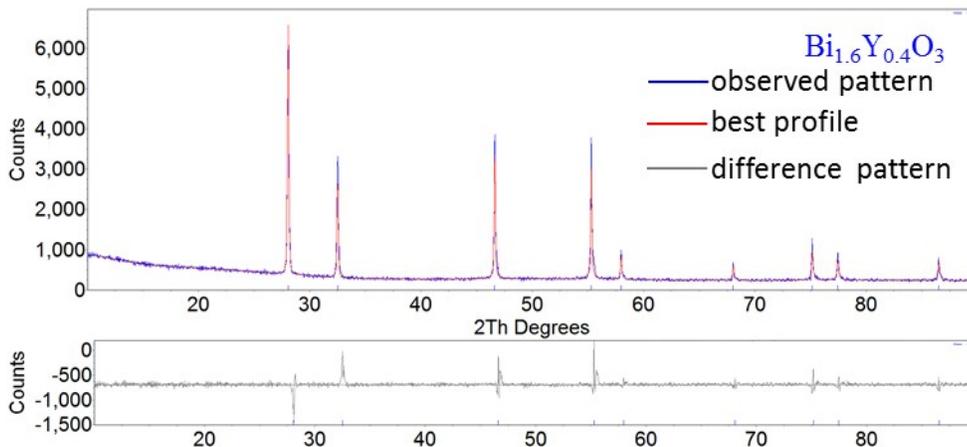
**Figure S4.** XRD patterns of  $(\text{Bi}_{1-x}\text{Y}_x)_2\text{O}_3$  ( $x$  is the mol percent of  $\text{Y}_2\text{O}_3$ ). Samples were sintered under 1273 K with 20h of reaction time and cooled in the air.

## Rietveld refinement

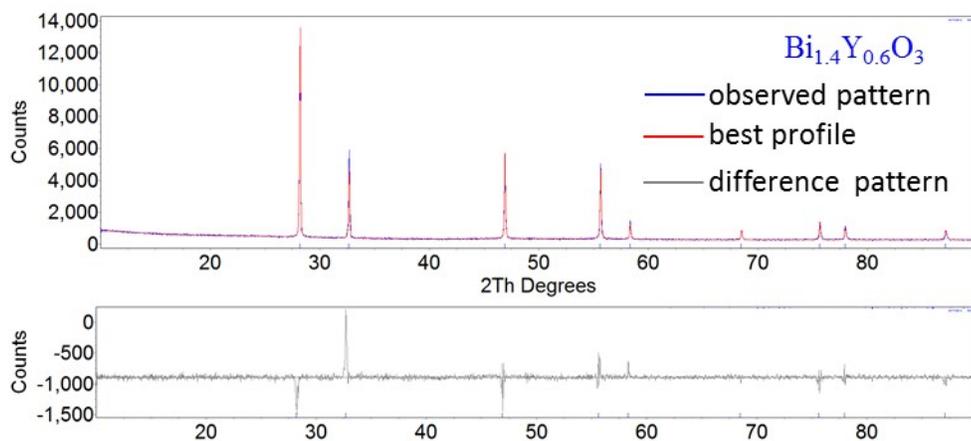
Table S1 is the summary of the results of Rietveld refinement. Figure S6-S12 show the Rietveld profiles refinement of the samples which are characterized as single phase by X-ray diffraction pattern comparison. The best Rietveld fit profiles and the difference curve between the observed and the calculated profiles are shown. The best fit to the data was validated by Rietveld refinement using the TOPAS program. The products have the same crystal structure in the space group of  $Fm\bar{3}m$  (225). Y and Bi atoms occupy 4a (0,0,0) site with a ratio depending on doping concentration. O ions are at 8c (0.25,0.25,0.25) site with a 0.75 occupancy.

**Table S1** Important results of Rietveld refinement (x indicates the nominal composition), the other information are included in the CIF file.

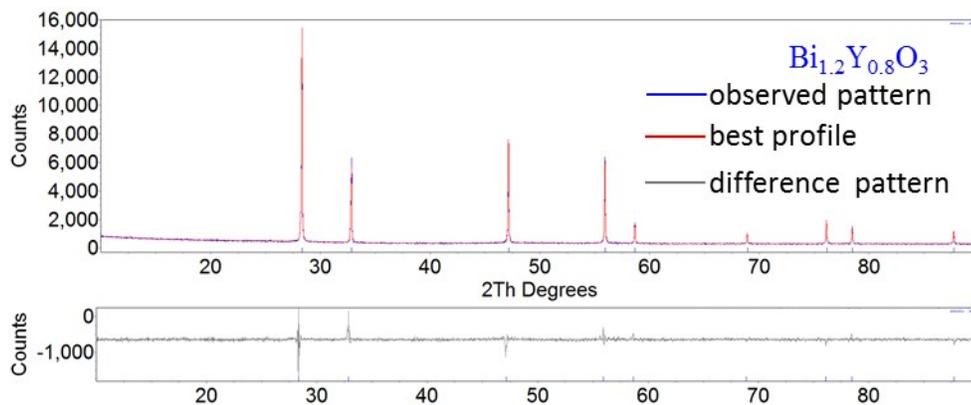
Temperature:293K; space group :Fm-3m(225,Cubic); radiation:Cu-K $\alpha$ ; wavelength:0.1540598nm; scan mode:2 $\theta$										
x	2 $\theta$ max (°)	step width (°2 $\theta$ )	Rietveld refinement information							
			a(Å)	$\rho_{\text{calc}}$ (g/cm $^3$ )	V(cm $^3$ )	R $_p$ (%)	R $_{\text{exp}}$ (%)	R $_{\text{wp}}$ (%)	R $_{\text{Bragg}}$ (%)	GOF=R $_{\text{wp}}$ /R $_{\text{exp}}$
x=0.2	90	0.026	5.506(2)	8.29(1)	166.92(1)	6.537	5.065	9.019	8.382	1.781
x=0.3			5.478(1)	8.05(2)	164.39(1)	5.643	4.719	7.527	6.528	1.595
x=0.4			5.447(1)	7.70(1)	161.63(2)	5.513	4.694	7.063	3.972	1.505
x=0.48			5.424(2)	7.26(2)	159.59(1)	5.694	4.368	7.514	6.346	1.72
x=0.5			5.418(1)	7.31(1)	159.02(1)	5.988	4.444	7.852	3.770	1.767
x=0.4		0.01	5.448(1)	7.58(1)	161.70(1)	4.938	6.025	6.255	2.275	1.038
x=0.48			5.426(1)	7.29(1)	159.72(1)	4.315	5.533	5.597	2.596	1.012



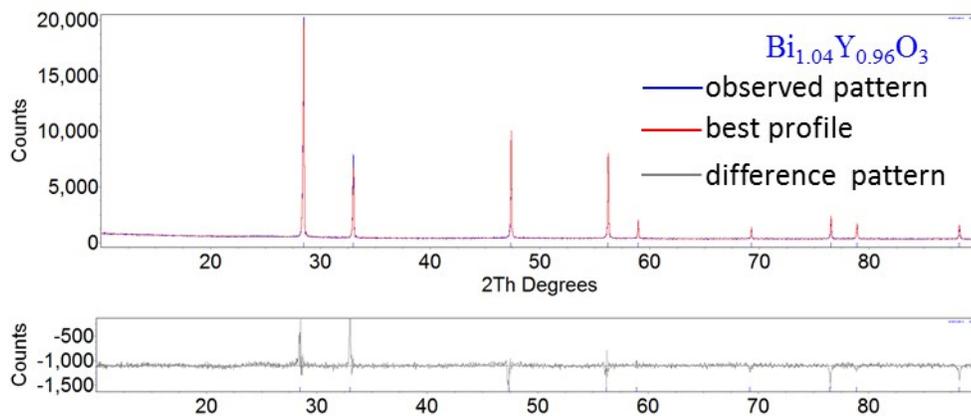
**Figure S5.** Rietveld refinement result of  $(\text{Bi}_{1-x}\text{Y}_x)_2\text{O}_3$  ( $x=0.2$ ) with  $0.026$  ( $^\circ$   $2\theta$ ) step width.



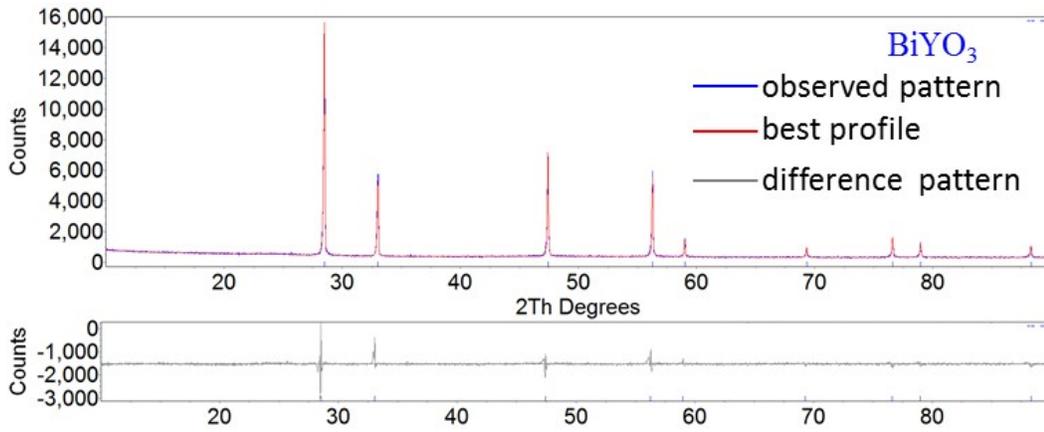
**Figure S6.** Rietveld refinement result of  $(\text{Bi}_{1-x}\text{Y}_x)_2\text{O}_3$  ( $x=0.3$ ) with  $0.026$  ( $^\circ$   $2\theta$ ) step width.



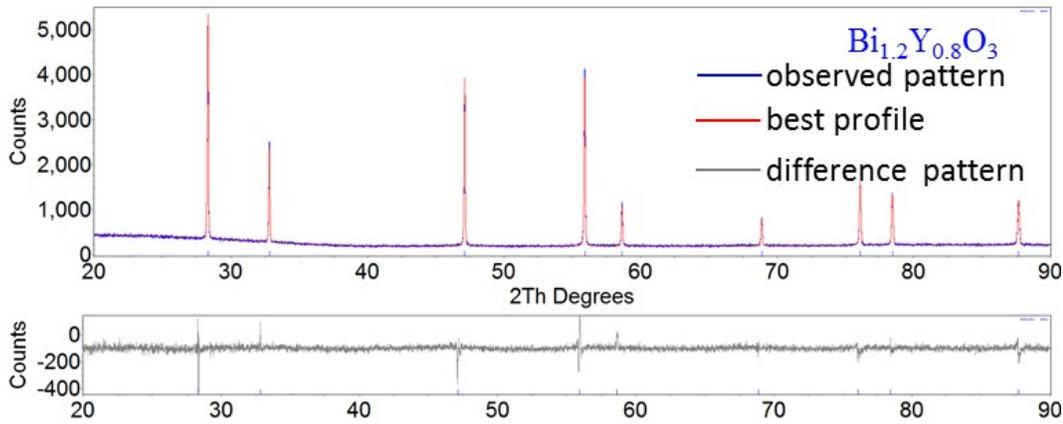
**Figure S7.** Rietveld refinement result of  $(\text{Bi}_{1-x}\text{Y}_x)_2\text{O}_3$  ( $x=0.4$ ) with  $0.026$  ( $^\circ$   $2\theta$ ) step width.



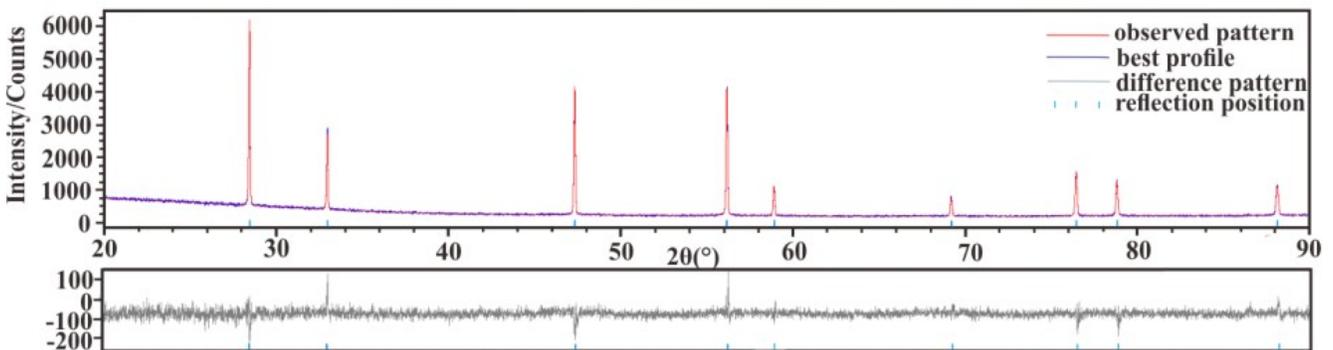
**Figure S8.** Rietveld refinement result of  $(\text{Bi}_{1-x}\text{Y}_x)_2\text{O}_3$  ( $x=0.48$ ) with  $0.026$  ( $^\circ$   $2\theta$ ) step width.



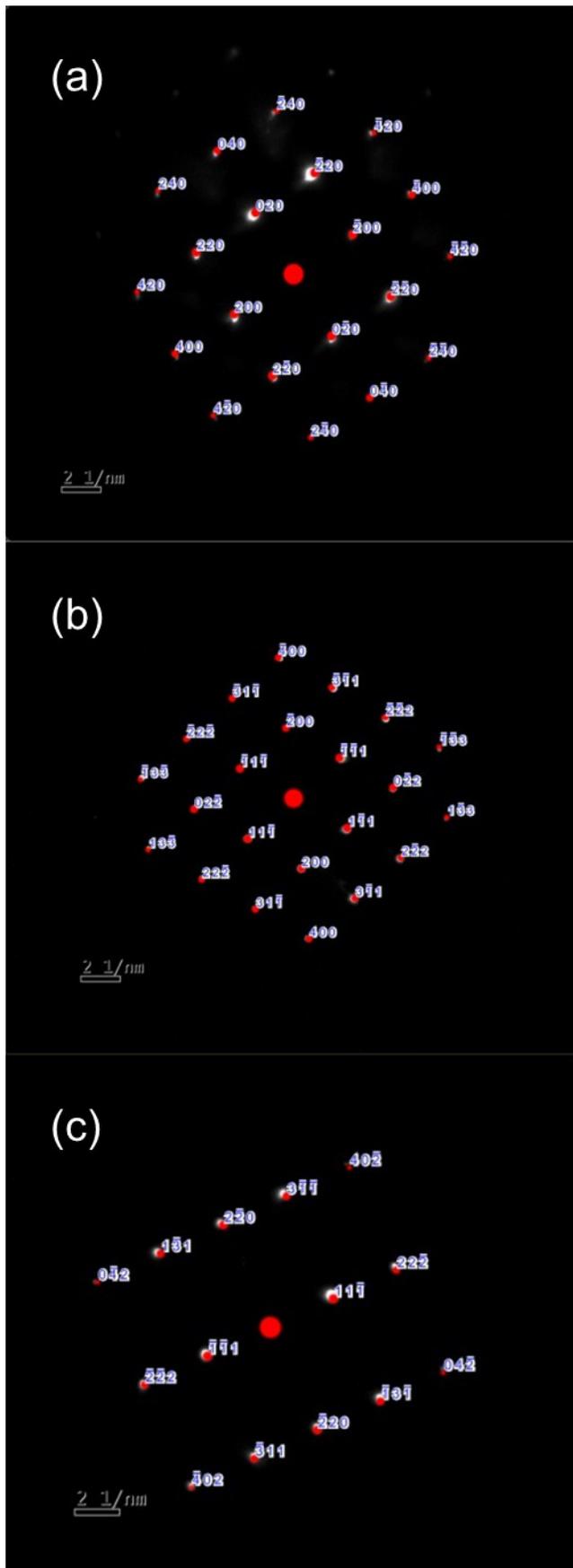
**Figure S9.** Rietveld refinement result of  $(\text{Bi}_{1-x}\text{Y}_x)_2\text{O}_3$  ( $x=0.5$ ) with  $0.026$  ( $^\circ$   $2\theta$ ) step width.



**Figure S10.** Rietveld refinement result of  $(\text{Bi}_{1-x}\text{Y}_x)_2\text{O}_3$  ( $x=0.4$ ) with  $0.01$  ( $^\circ$   $2\theta$ ) step width.



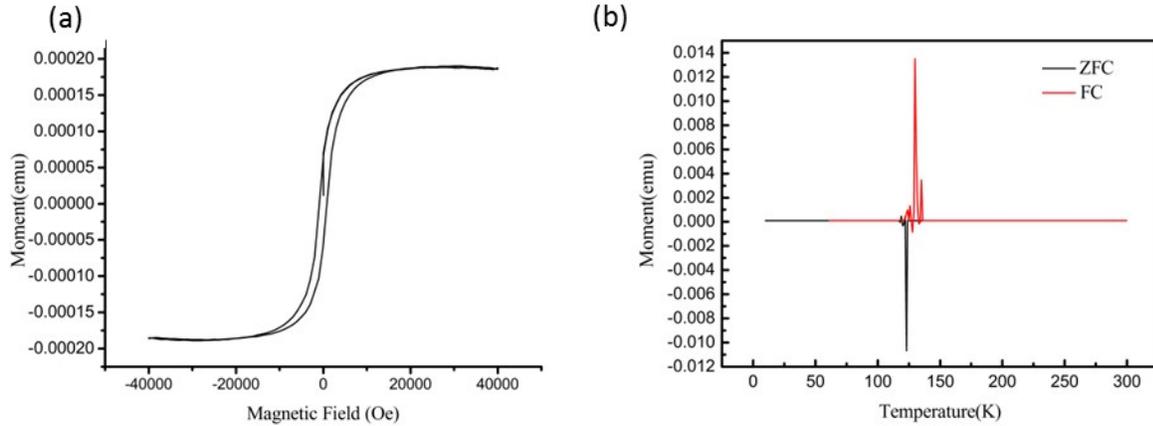
**Figure S11.** Rietveld refinement result of  $(\text{Bi}_{1-x}\text{Y}_x)_2\text{O}_3$  ( $x=0.48$ ) with  $0.01$  ( $^\circ$   $2\theta$ ) step width.



**Figure S12.** Electron diffraction pattern of the BiYO<sub>3</sub> sample with an incident electron beam along different view direction. (a): [001] direction; (b): [011] direction;(c): [112] direction (The red dots are the simulation of electron diffraction with the structure of BiYO<sub>3</sub> obtained by Rietveld refinement .)

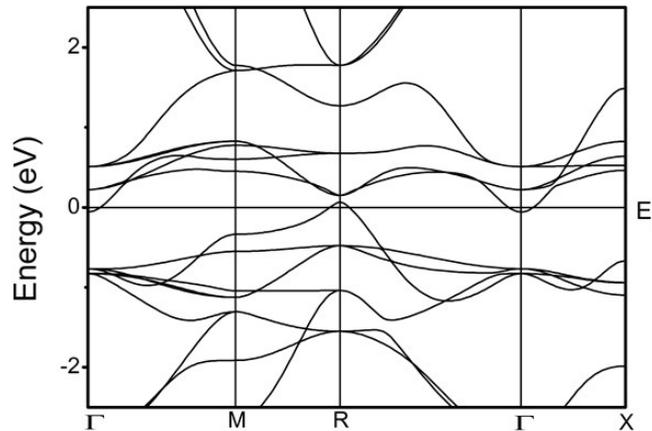
## PPMS (physical property measurement system)

In Figure S13, none of any magnetic signal was observed for the  $x=0.48$  sample with PPMS.



**Figure S13.** The results for the  $x=0.48$  sample with PPMS. (a) The curve of magnetic field and the magnetic moment ( $T=10\text{K}$ ); (b) The curve of temperature and magnetic moment ( $H=0.2\text{T}$ )

## Band structure



**Figure S14.** Band structure of the "perovskite"  $\text{YBiO}_3$  without spin orbit coupling

## Crystal data used for computations

- 1) High pressure phase, Perovskite structure

**Experimental:** Pm-3m,  $a=4.2 \text{ \AA}$  (Ref.[12] and Database below)

Y: (0, 0, 0); Bi: (0.5, 0.5, 0.5); O: (0.5, 0, 0)

([http://materials.springer.com/isp/crystallographic/docs/sd\\_0550507](http://materials.springer.com/isp/crystallographic/docs/sd_0550507))

**Optimized:** Pm-3m, a=4.283 Å (Our VASP calculations)

Y: (0, 0, 0); Bi: (0.5, 0.5, 0.5); O: (0.5, 0, 0)

2) “High pressure” phase, “Perovskite” structure

**Experimental:** Pm-3m, a=5.428 Å (Ref.[14] and Database below)

Y: (0, 0, 0); Bi: (0.5, 0.5, 0.5); O: (0.0, 0.5, 0.5)

([http://materials.springer.com/isp/crystallographic/docs/sd\\_0304073](http://materials.springer.com/isp/crystallographic/docs/sd_0304073))

**Optimized:** Pm-3m, a=4.373 Å(Our VASP calculations)

Y: (0, 0, 0); Bi: (0.5, 0.5, 0.5); O: (0.0, 0.5, 0.5)

3) Ambient pressure, Pyrochlore structure

**Experimental:** Fd-3m, a=11.55 Å (Ref. [12] and Database below)

Y: (0, 0, 0); Bi: (0.5, 0.5, 0.5); O: (0.305, 1/8, 1/8)

([http://materials.springer.com/isp/crystallographic/docs/sd\\_1102208](http://materials.springer.com/isp/crystallographic/docs/sd_1102208))

**Optimized:** Fd-3m, a=10.913 Å (Our VASP calculations)

Y: (0, 0, 0); Bi: (0.5, 0.5, 0.5); O: (0.3642, 1/8, 1/8)