Electronic Supplementary Information (ESI)

Bismuth-iron-based Precursor: Preparation, Phase composition, and its Thermal Treatment in Two Ways

Yunpeng Liu,[ab] Hao Wang,[ab] Lixiong Qian,[ab] Xiaoyi Zhao,[ab] Lei Yao,[a] Jiayi Wang,[a] Xueqing Xing,[a] Guang Mo[a], Zhongjun Chen,[a] Zhonghua Wu[ab]*

[a]Institute of High Energy Physics, Chinese Academy of Sciences, Beijing 100049, China

[b]University of Chinese Academy of Sciences, Chinese Academy of Sciences,Beijing 100049, China

***: Correspondence to:** Zhonghua Wu, E-mail: wuzh@ihep.ac.cn

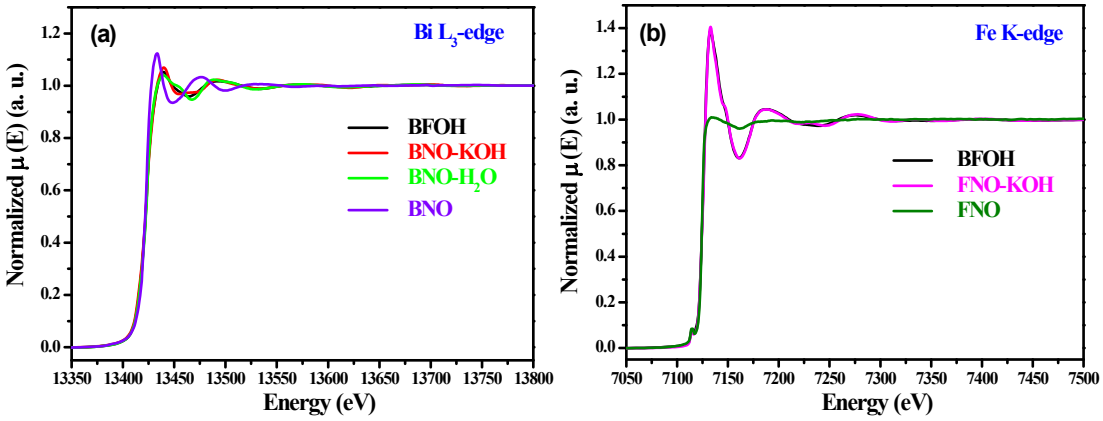

Figure S1. X-ray absorption fine structure (XAFS) spectra of the as-prepared samples BFOH, BFO-KOH, BFO-H_2O, BNO, FNO-KOH and FNO. (a) Bi L_3-edge; (b) Fe K-edge.

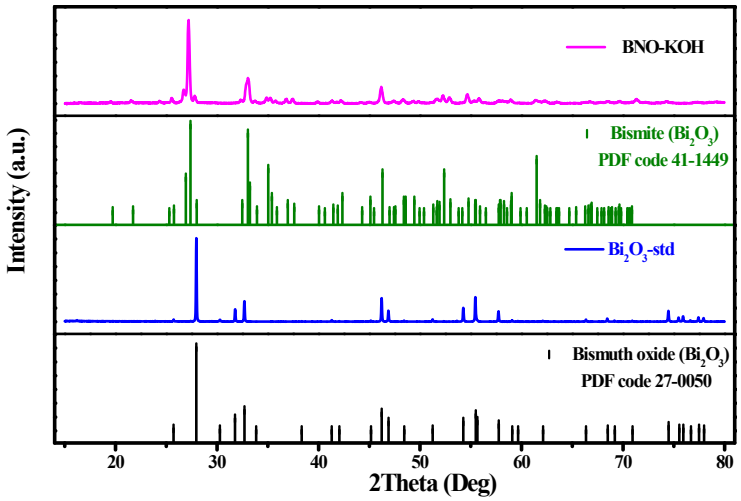

Figure S2. XRD patterns of the purchased standard sample Bi_2O_3-std (β-Bi_2O_3) and as-prepared BNO-KOH (α-Bi_2O_3). Two reference XRD patterns of $Bi_2O_3$are also given.

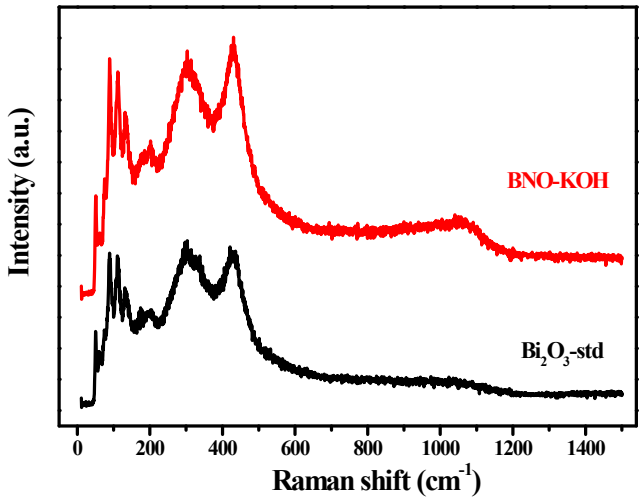

Figure S3. Raman spectra of the purchased standard sample Bi_2O_3-std (β-Bi_2O_3) and the as-prepared BNO-KOH (α-Bi_2O_3).

Figure S4. Photographs of the purchased sample Bi_2O_3-std (β-Bi_2O_3) and as-prepared BNO-KOHpowders (α-Bi_2O_3).

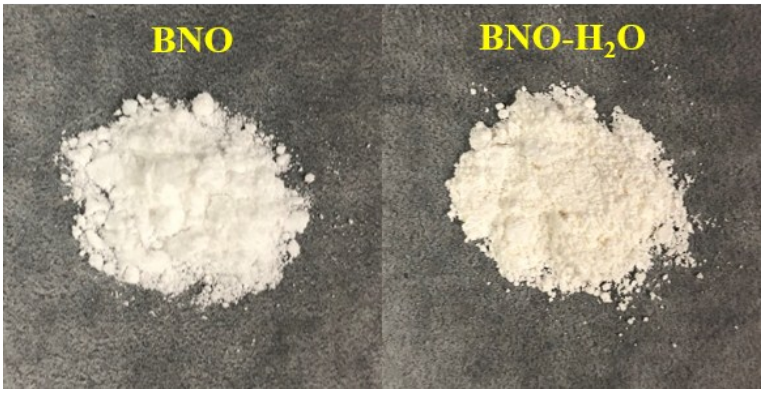

Figure S5. Photographs of the BNO ($Bi(NO_3)_3 \cdot 5H_2O$) and as-prepared BNO-H_2O powders ($Bi_6O_5(NO_3)_5(OH)_3 \cdot 3H_2O$ and $Bi_6O_6(NO_3)_4(OH)_2 \cdot 2H_2O$ mixture).

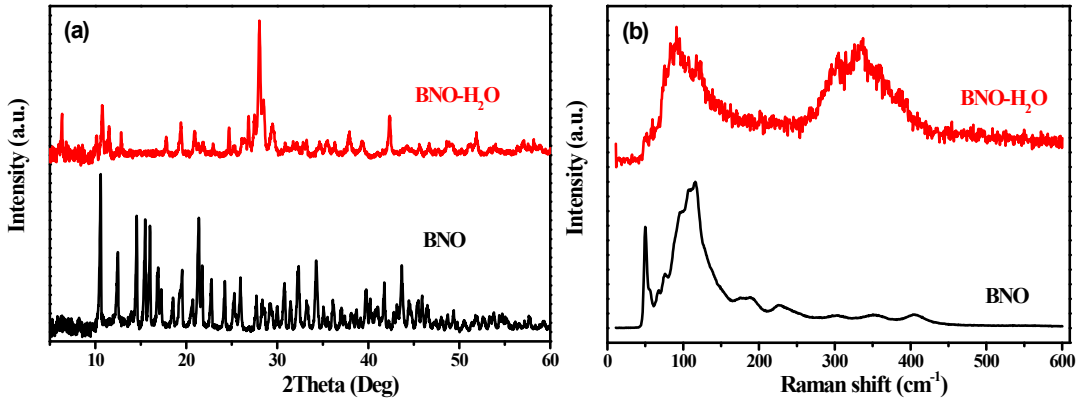

Figure S6. XRD patterns (a) and Raman spectra (b) of the BNO and as-prepared BNO-H_2O.

Figure S7. Photographs of the as-prepared BNO-KOH (α-Bi_2O_3), FNO-KOH ($Fe(OH)_3$), BFOH, and BNO-H_2O($Bi_6O_5(NO_3)_5(OH)_3 \cdot 3H_2O$ and $Bi_6O_6(NO_3)_4(OH)_2 \cdot 2H_2O$ mixture) powders.

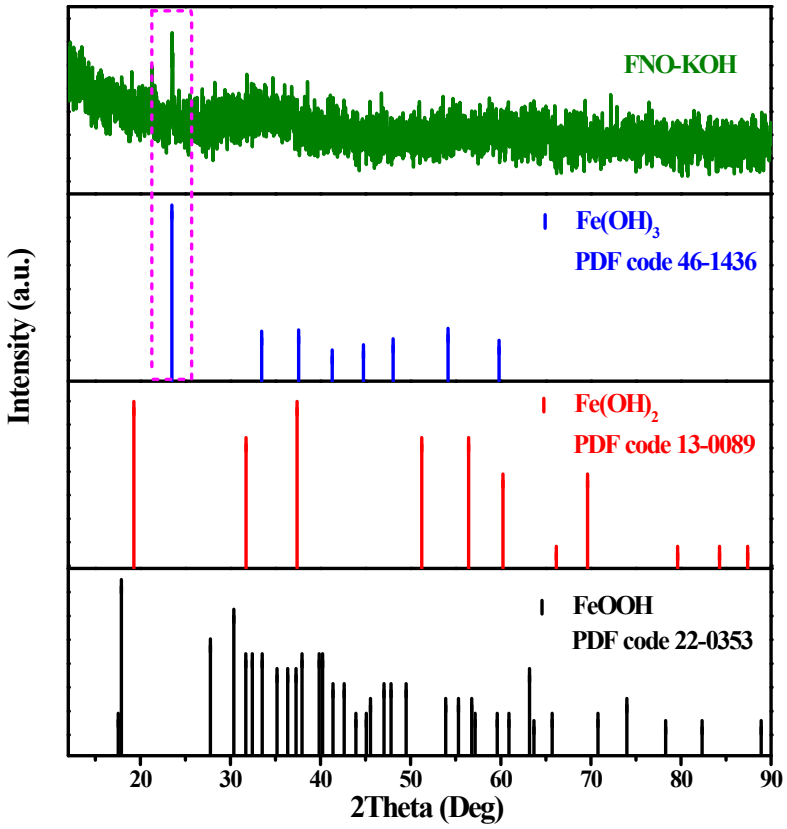

Figure S8. XRD pattern comparison between the as-prepared FNO-KOH ($Fe(OH)_3$) sample and the references (PDF code 46-1436, PDFcode 13-0089, and PDF code 22-0353).

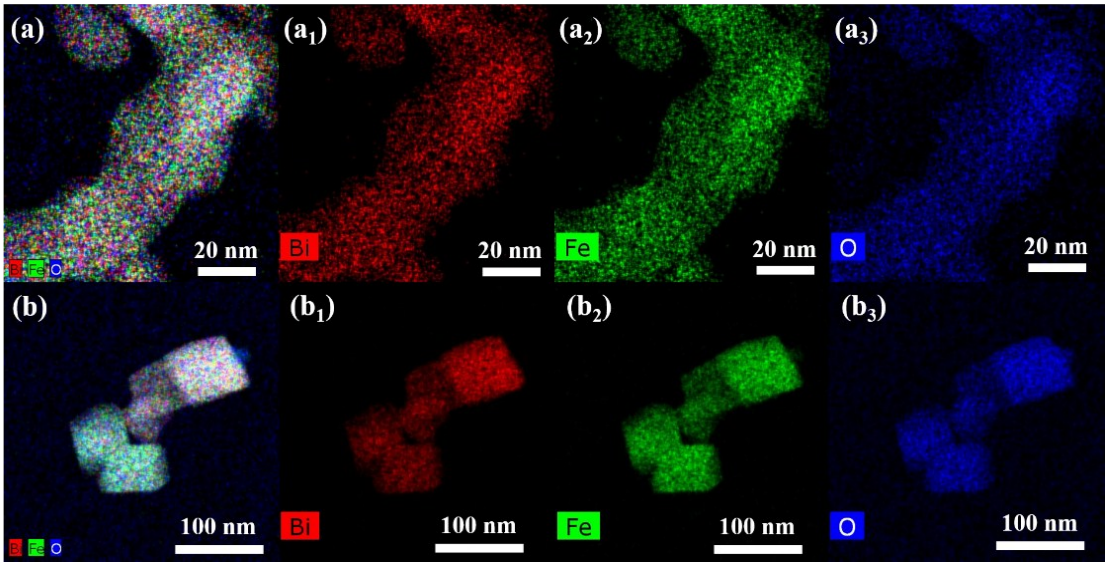

Figure S9. Mapping of Bi, Fe, and O element distributions in samples BFOH-400°C (a) and BFOH-500°C (b).

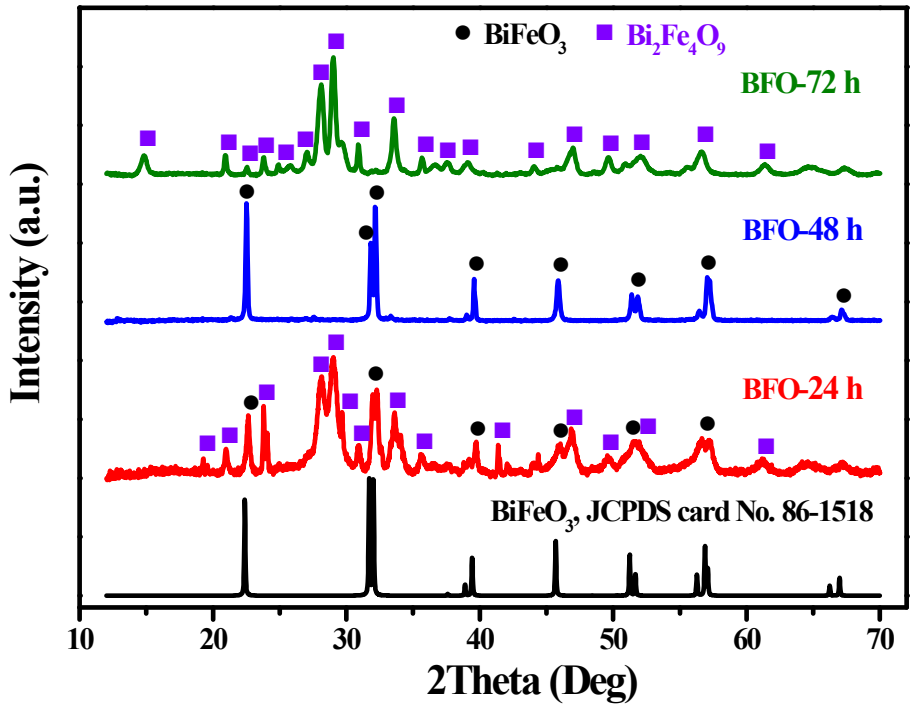

Figure S10. XRD patterns of the hydrothermal synthesized samples BFO-24h, BFO-48h, and BFO-72h.

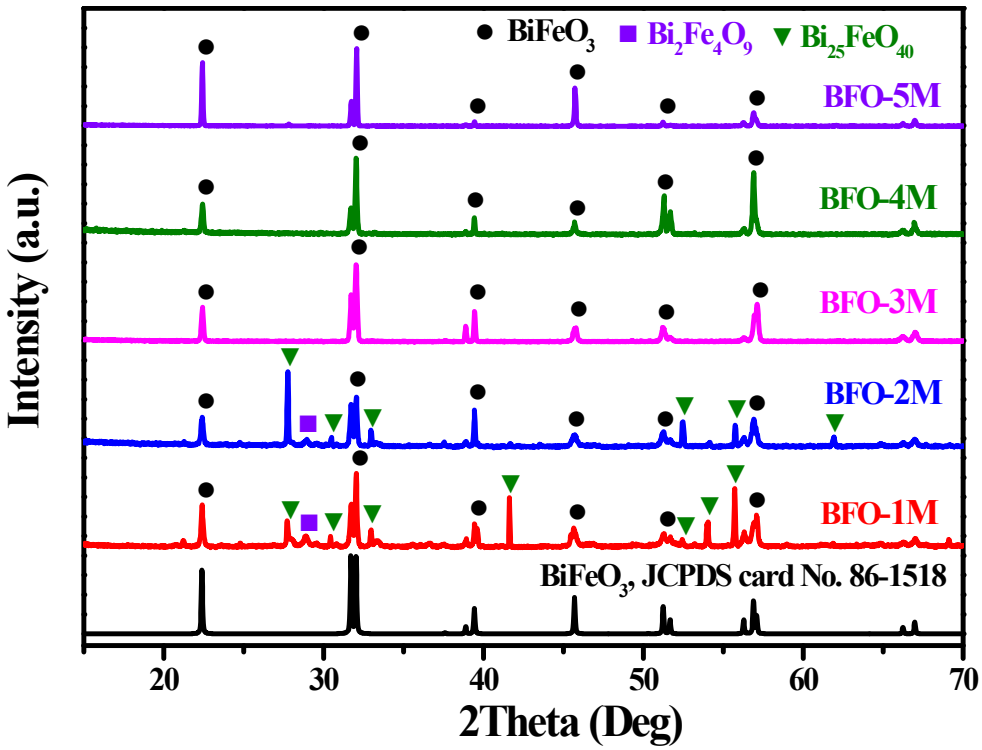

Figure S11. XRD patterns of the hydrothermal synthesized samples BFO-1M, BFO-2M, BFO-3M, BFO-4M, and BFO-5M.

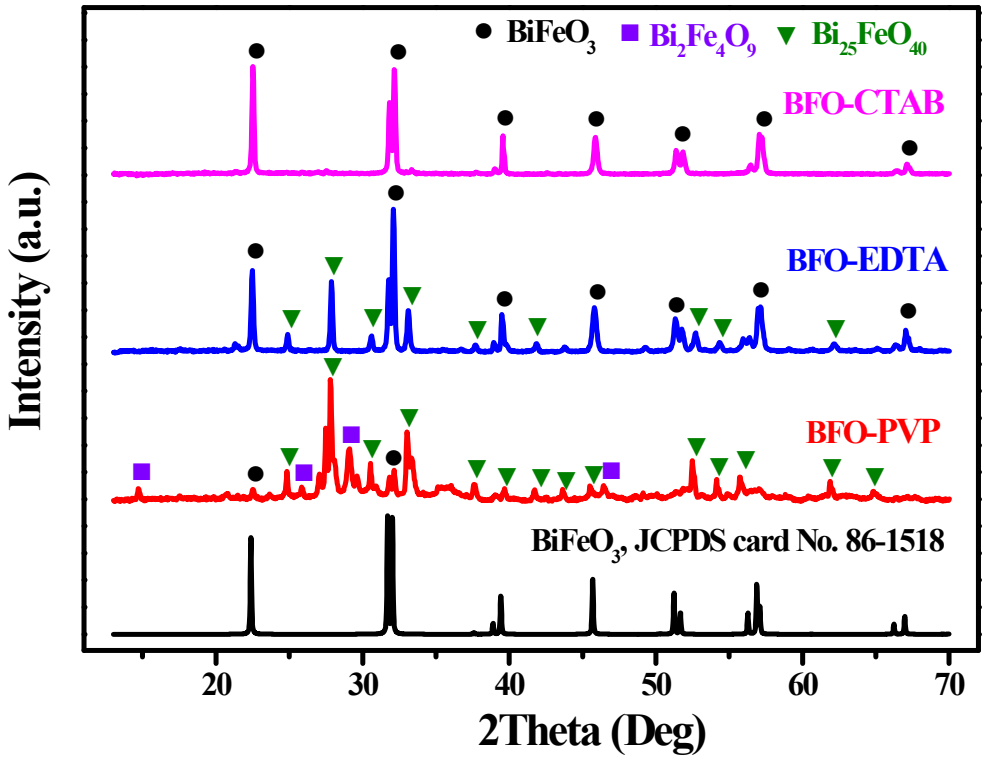

Figure S12. XRD patterns of the hydrothermal synthesized samples BFO-PVP, BFO-EDTA, and BFO-CTAB.

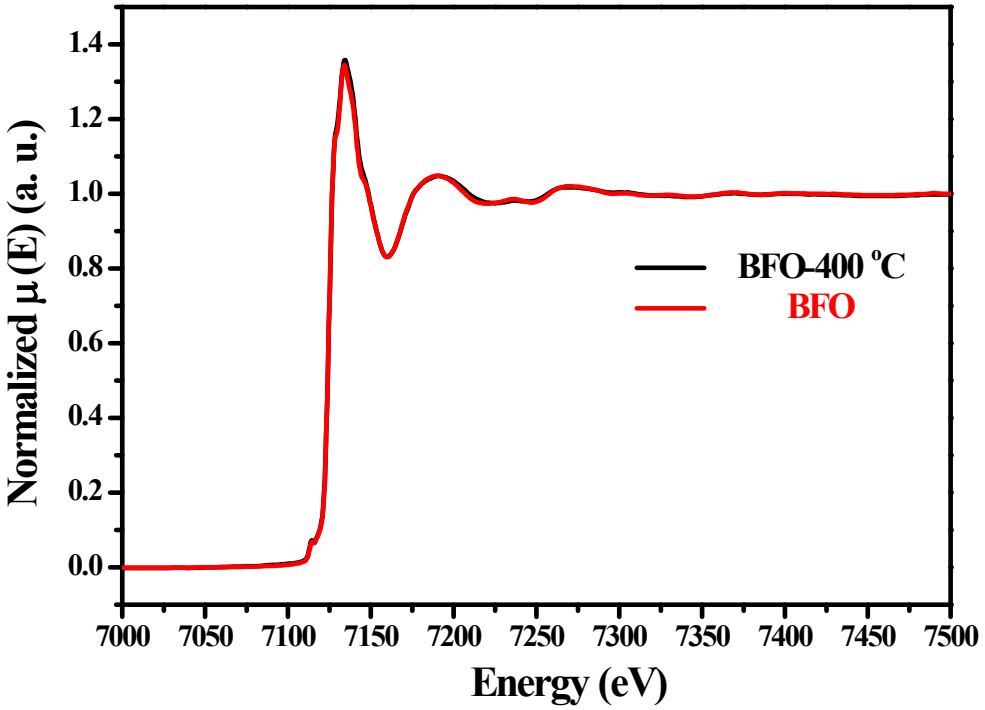

Figure S13. Fe K-edge X-ray absorption spectra of the as-prepared samples BFO-400°C and BFO.

Table S1. Bi L_3-edge EXAFS fitting parameters of sample BFO-400°C and BFO.

Sample	Bond	R (Å)	N	σ^2 (10^{-3} Å^2)	ΔE (eV)
$BiFeO_3$[s1]	Bi-O	2.314	3		
	Bi-O	2.523	3		
	Bi-O	3.210	3		
	Bi-Fe	3.313	3		
	Bi-Fe	3.581	3		
BFO-400°C	Bi-O	2.16	3.1	6	-9.3
	Bi-O	2.34	0.4	6	-9.3
	Bi-O	3.00	2.9	6	-9.3
	Bi-Fe	3.38	2.8	8	6.7
	Bi-Fe	3.60	3.2	8	6.7
BFO	Bi-O	2.18	3.2	5	-8.3
	Bi-O	2.33	0.4	5	-8.3
	Bi-O	3.00	2.9	5	-8.3
	Bi-Fe	3.37	3.1	7	4.4
	Bi-Fe	3.59	2.9	7	4.4

References:

s1. J. M.Moreau, C.Michel, R.Gerson, and W. J.James, *J. Phys. Chem. Solids* 1971, **32**, 1315-1320.