

Supplementary Information

Low temperature synthesis of BiFeO₃ nanoparticles with enhanced magnetization and promising photocatalytic performance in dye degradation and hydrogen evolution

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Table-S1: Rietveld Refined structural parameters and phases present (in wt %) obtained from powder XRD

Sample	Crystal Structure	Lattice Parameters (Å)	Atomic Coordinates	R Factor
BFO Bulk	BFO(R3c) (Rhombohedral) Fract (%): 79.79(0) Vol: 373.370(0.004)	a=b=5.5764(2) c=13.8640(1)	Bi (0,0,0) Fe (0,0, 0.2202) O(0.4478, 0.0006, 0.9545)	$\chi^2 = 2.30$ $R_p = 1.21$ $R_{wp} = 1.69$
	Bi ₂ Fe ₄ O ₉ (pbam) (Orthorhombic) Fract(%): 8.69 (0) Vol: 404.169(0.035)	a =8.4433(4) b=7.9723(4) c=6.0043(3)	Bi (0.17524, 0.17916, 0) Fe1 (0.5, 0, 0.27910) Fe2 (0.35714, 0.35660,0.5) O1 (0, 0, 0.5) O2(0.27003, 0.73403,-0.34894) O3 (0.83303, 0.72656, 0.5) O4(0.46749, 0.13604, 0.88808)	
	BFO(pnma) (Orthorhombic) Fract (%): 4.86(0) Vol: 99.962(0.063)	a=3.6953(6) b=4.1502(15) c=6.517(3)	Bi (0.07672, -0.54738, -0.10374) Fe (0.64829, 0.72185, 0.62450) O1 (-0.29397, 0.39633, -0.14315) O2 (0.26305, -0.27487, -0.34784) O3 (0.08274, -0.34590, 0.07061)	
	Bi ₂₅ FeO ₄₀ (I23) (Cubic) Fract(%): 6.66(0) Vol: 1050.261(0.072)	a=b=c= 10.1648(4)	Bi (0.69420, -0.87266, 0.57740) Bi/Fe (0,0,0) O1(0.10396, 0.10328, 0.29397) O2 (0.69383, -0.50582, 0.22787) O3(0.75608, 0.75608, 0.75608)	
Bi _{12.5} Fe _{0.5} O _{19.5} 120°C	Bi _{12.5} Fe _{0.5} O _{19.5} (I23) (Cubic) Fract(%): 50.23(0.62) Vol:1049.414(0.049)	a=b=c= 10.1620(3)	Bi1 (0.1782, 0.3149, 0.0139) Fe (0,0,0) Bi2 (-0.0310, -0.0310, -0.0310) O1 (0.1336, 0.2364, 0.5141) O2 (0.1694, 0.1694, 0.1694) O3 (0.8937, 0.8937, 0.8937)	$\chi^2 = 1.37$ $R_p = 3.52$ $R_{wp} = 4.82$

	Bi ₂ O ₃ (P121/c) (Monoclinic) Fract(%): 49.40(0.88) Vol: 328.746(0.025)	a=5.8406(3) b=8.1557(3) c=7.4977(4)	Bi1 (0.5257, 0.1885, 0.6384) Bi2 (0.0379, 0.0424, 0.2253) O1 (0.6150, 0.2780, 0.3160) O2 (0.6481, -0.0095, 0.0945) O3 (0.0189, 0.0918, 0.4769)	
Bi ₂ O ₃ 140°C	Bi _{12.5} Fe _{0.5} O _{19.5} (I2 3) (Cubic) Fract(%): 29.98(0.32) Vol:1050.125(0.0 36)	a=b=c= 10.1643(2)	Bi1 (0.1775, 0.3132, 0.0109) Fe (0,0,0) Bi2 -0.0205, -0.0205, -0.0205) O1 (0.1257, 0.2617, 0.5488) O2 (0.1778, 0.1778, 0.1778) O3 (0.8892, 0.8892, 0.8892)	$\chi^2 = 1.18$ $R_p = 3.87$ $R_{wp} = 4.92$
	Bi ₂ O ₃ (P121/c) (Monoclinic) Fract(%): 70.02(0.55) Vol: 329.463(0.020)	a=5.8443(2) b=8.1618(2) c=7.5053(3)	Bi1 (0.5296, 0.1835, 0.6368) Bi2 (0.0418, 0.0421, 0.2201) O1 (0.6377, 0.2910, 0.3843) O2 (0.7170, -0.0619, 0.1571) O3 (0.0189, 0.0918, 0.4769)	
BFO 160°C	BFO (R3c) (Rhombohedral) Fract(%): 100(0) Vol: 373.327(0.014)	a = b =5.5758(1) c =13.8656(4)	Bi (0,0,0) Fe (0,0, 0.2215) O (0.4598, 0.0184, 0.9519)	$\chi^2 = 1.75$ $R_p = 5.58$ $R_{wp} = 7.27$
BFO 180°C	BFO (R3c) (Rhombohedral) Fract(%): 98.24(0.01) Vol: 373.314(0.01)	a = b =5.5761(1) c =13.8634(3)	Bi (0,0,0) Fe (0,0, 0.2198) O (0.4694, 0.0247, 0.95)	$\chi^2 = 1.54$ $R_p = 5.42$ $R_{wp} = 7.19$
BFO 200°C	BFO(R3c) (Rhombohedral) Fract (%): 100(0) Vol: 373.24(0.085)	a = b =5.5754 (1) c =13.8645 (4)	Bi (0,0,0) Fe (0,0, 0.2248) O (0.4556, 0.0238, 0.9398)	$\chi^2 = 1.93$ $R_p = 5.85$ $R_{wp} = 7.64$