

Bandgap engineering strategy through chemical strain and oxygen vacancy in super-tetragonal BiFeO₃ epitaxial films

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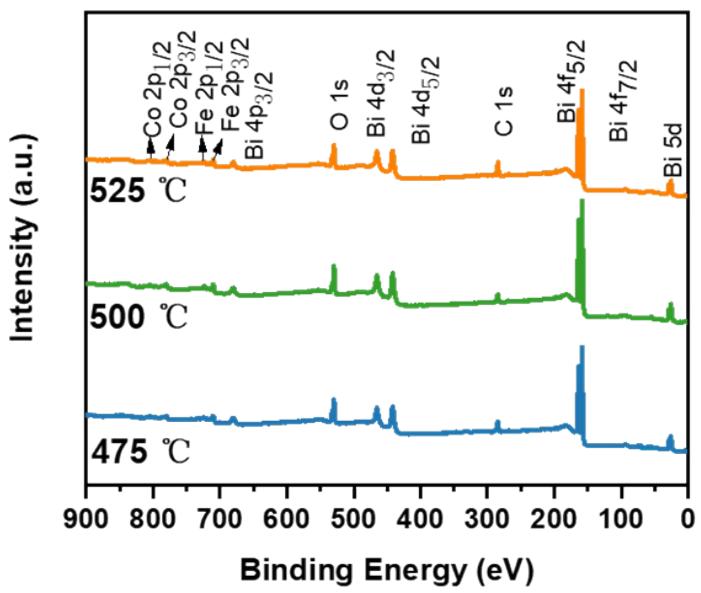


Figure S1 XPS full spectrum of BFCO₂ films grown at different temperatures on LAO (100) substrates.

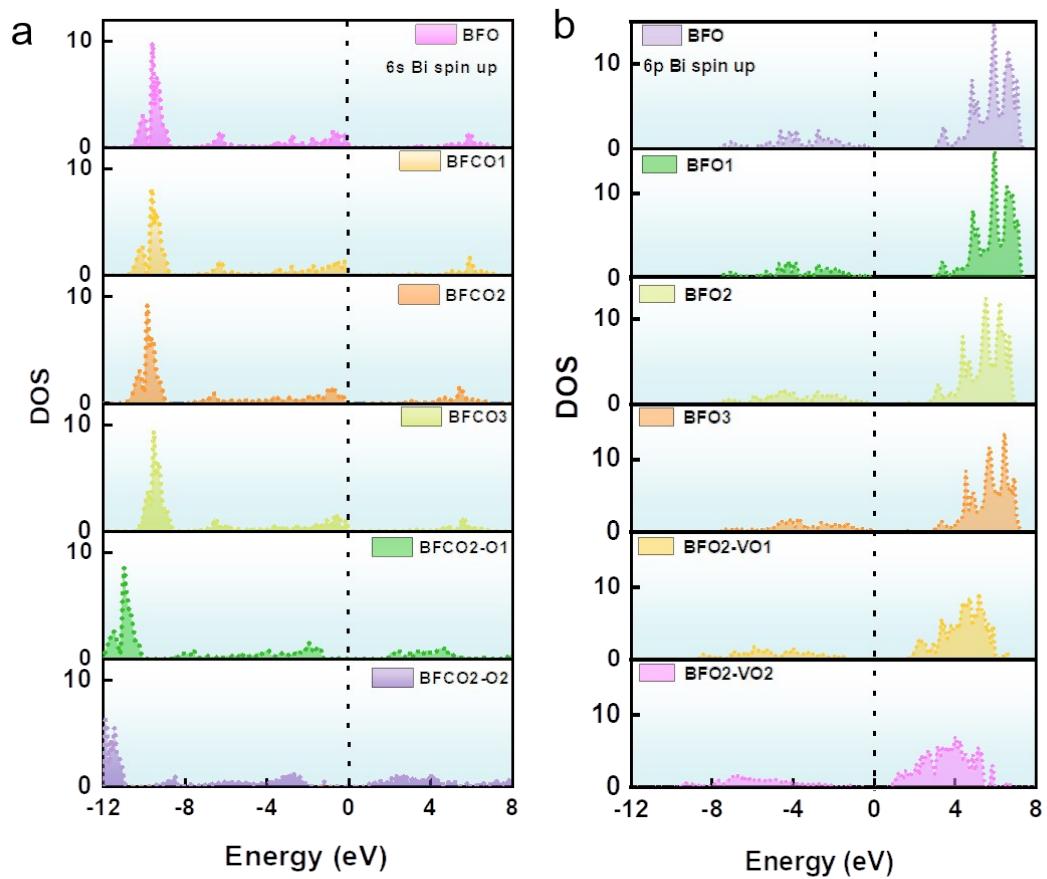


Figure S2 (a) Bi 6s DOS of $\text{BiFe}_x\text{Co}_{1-x}\text{O}_3$ and $\text{BFO}_2\text{-Vac(O}_1\text{)}$ or $\text{BFO}_2\text{-Vac(O}_2\text{)}$. **(b)** Bi 6p DOS of $\text{BiFe}_x\text{Co}_{1-x}\text{O}_3$ and $\text{BFO}_2\text{-Vac(O}_1\text{)}$ or $\text{BFO}_2\text{-Vac(O}_2\text{)}$.

Table S1 Fe and Co contents of BFCO2 films grown at different temperatures

Temperature (°C)	Fe (atom%)	Co (atom%)	Co%
525	8.53	3.26	27.64%
500	5.34	3.2	37.47%
475	6.17	4.33	41.23%

Table S2. Fe²⁺ (Fe³⁺), Co²⁺ (Co³⁺), and oxygen vacancies contents of BFCO2 films

grown at different temperatures

Temperature (°C)	Co ^{2+:} Co ³⁺ (area ratio)	Fe ^{2+:} Fe ³⁺ (area ratio)	V _{ac:} Lat (area ratio)
525	0.28	0.43	0.11
500	0.32	0.59	0.13
475	0.66	0.81	0.24