

Supplementary Information

Experimental Visualization of the Bi-O Covalency in Ferroelectric Bismuth Ferrite BiFeO₃ by Synchrotron X-ray Powder Diffraction Analysis

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The refined atomic coordinates of BiFeO₃

	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> (Å ²)
Bi	6a	0	0	0	0.00988(4)
Fe	6a	0	0	0.22106(8)	= <i>U</i> (Bi)
O	18b	0.4532(8)	0.0265(7)	0.9558(3)	= <i>U</i> (Bi)

Fractional atomic coordinates used in the Figures 2b

	<i>x</i>	<i>y</i>	<i>z</i>	Symmetry Operation
Fe	1/3	2/3	0.3877	- <i>y</i> +1/3, - <i>x</i> +2/3, <i>z</i> +1/6
O _a	0.4532	0.4267	0.4558	<i>x</i> , <i>x</i> - <i>y</i> , <i>z</i> -1/2
O _b	0.6402	0.7600	0.2892	- <i>y</i> +2/3, <i>x</i> - <i>y</i> +1/3, <i>z</i> +1/3

Fractional atomic coordinates used in the Figures 2c

	<i>x</i>	<i>y</i>	<i>z</i>	Symmetry Operation
Bi	2/3	1/3	1/3	<i>x</i> +2/3, <i>y</i> +1/3, <i>z</i> +1/3
O _a	0.4532	0.4267	0.4558	<i>x</i> , <i>x</i> - <i>y</i> , <i>z</i> +1/2
O _b	0.6402	0.7600	0.2892	- <i>y</i> +2/3, <i>x</i> - <i>y</i> +1/3, <i>z</i> -2/3
O _c	0.1199	0.3599	0.2892	<i>x</i> -1/3, <i>y</i> +1/3, <i>z</i> -2/3
O _d	0.9066	0.6932	0.1225	- <i>x</i> + <i>y</i> +4/3, <i>y</i> +2/3, <i>z</i> -5/6