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Temperature induced structural and polarization features in $BaFe_{12}O_{19}$

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SUPPLEMENTARY INFORMATION

TABLE T1. Rietveld refinement parameters obtained from the NPD for $BaFe_{12}O_{19}$ at 40 and 290 K and optimized by the first principal calculations.

		Exp 40 K	Exp 290 K	HSE (1/4, 3/4)	HSE (0.258, 0.758)
Ba (2d)	*z*	1/4	1/4	1/4	0.2490
Fe1 (2a)	*z*	0	0	0	0.0003
Fe2 (2a)	*z*	1/4	1/4	1/4	0.2579
Fe3 ($4f_{IV}$)	*z*	0.0256(9)	0.0278(6)	0.0272	0.0272
Fe4 ($4f_{VI}$)	*z*	0.1917(8)	0.1897(5)	0.1903	0.1904
Fe5 (12k)	*x*	0.1703(34)	0.1775(26)	0.1686	0.1694
	z	-0.1072(4)	-0.1082(3)	-0.1082	-0.1077
O1 (4e)	*z*	0.1592(16)	0.1548(11)	0.1508	0.1487
O2 (4f)	*z*	-0.0618(16)	-0.0569(11)	-0.0547	-0.0548
O4 (12k)	*x*	0.1527(44)	0.1538(28)	0.15674	0.1572
	z	0.0514(6)	0.0524(4)	0.0519	0.0515
O5 (12k)	*x*	0.5149(42)	0.5163(30)	0.5021	0.5019
	z	0.1490(7)	0.1513(5)	0.1491	0.1493
Relevance factors	R_{wp}, %	9.98	7.01		
	R_{exp}, %	3.83	3.98		
	R_B, %	9.34	2.74		
	R_{Mag}, %	3.90	1.47		
	χ^2	6.80	3.10		

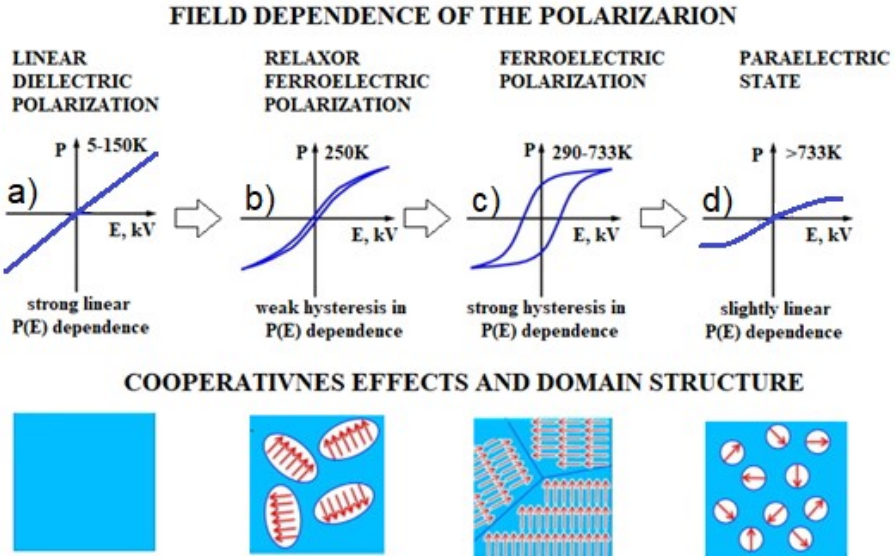


FIG. S1 Schematic illustration of the P(E) and domain structure behavior at different temperatures.

TABLE T2. Charge redistribution among ions in $BaFe_{12}O_{19}$

Ba	Fe1	Fe2	Fe3	Fe4	Fe5	O
$1.64e^-$	$1.92e^-$	$1.76e^-$	$1.84e^-$	$1.94e^-$	$1.90e^-$	$1.25e^-$ - $1.30e^-$

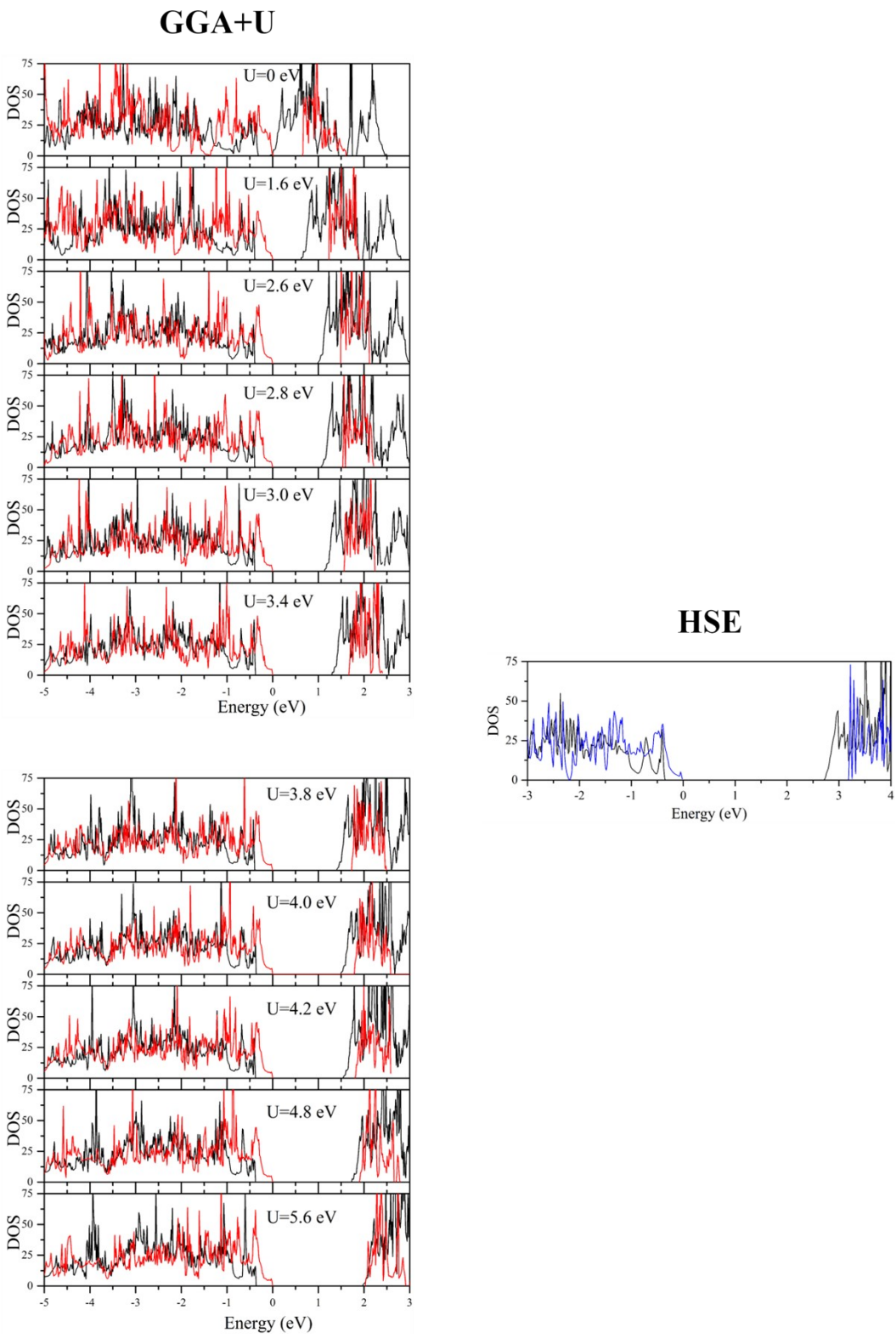


FIG. S2. Total density of states of $BaFe_{12}O_{19}$ as calculated by HSE and GGA+U (0 eV< U < 5.6 eV) for different spin polarization. Zero at the energy scale corresponds to the top of the valence band.

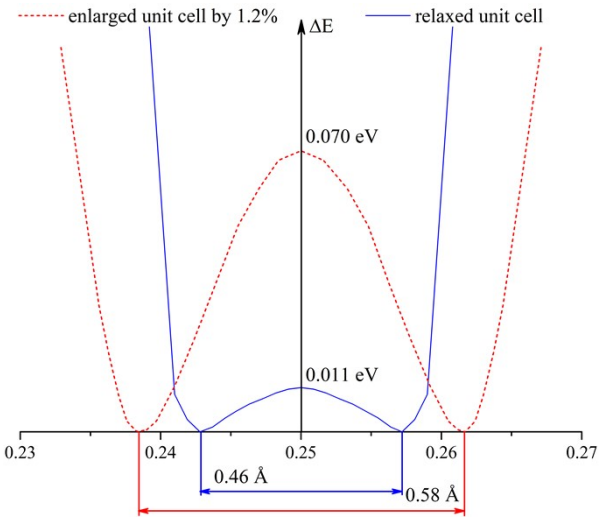


FIG. S3. The potential relief for the Fe2 ions around z=1/4 (z=3/4) for the fully relaxed and enlarged in volume unit cells by NEB within GGA+U with U=2.8 eV when moving two Fe2 atoms. The energy barriers and the distance of the Fe2 ion shift are indicated.

TABLE T3. Changes in atomic positions and interatomic distances in the FeO_5 trigonal bipyramid with the displacement of the Fe atom from z=1/4 to z=0.259.

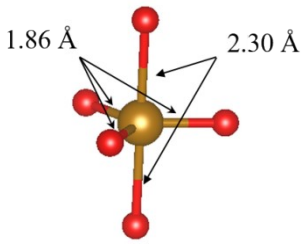
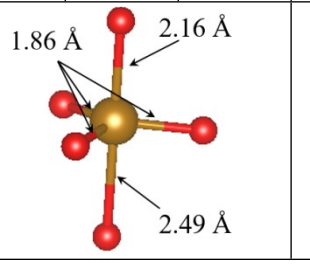
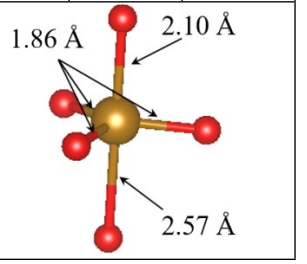
		z=1/4			z=0.256			z=0.259		
		x	y	z	x	y	z	x	y	z
	Fe2	0	0	1/4	0	0	0.256	0	0	0.259
equatorial	O	0.182	0.364	1/4	0.182	0.363	0.251	0.181	0.362	0.251
	O	0.182	0.818	1/4	0.182	0.818	0.251	0.181	0.819	0.251
	O	0.636	0.818	1/4	0.637	0.818	0.251	0.637	0.819	0.251
polar	O	0	0	0.151	0	0	0.149	0	0	0.149
	O	0	0	0.349	0	0	0.349	0	0	0.349
										

TABLE T4. Atomic coordinates of $BaFe_{12}O_{19}$ determined with the Rietveld method in the framework of: SG *P6₃/mmc* (#194), SG *P6₃mc* (#186) and SG *P6₃22* (#182).

Composition / Atomic positions	SG#194		SG#186		SG#182	
	T, K					
	40 K	290 K	40 K	290 K	40 K	290 K
Ba	**(2d)**		**(2b)**		**(2d)**	
z	0.25	0.25	0.2427(70)	0.2501(83)	0.25	0.25
Fe1 (2a)						
z	0	0	-0.0108(45)	-0.0089	0	0
Fe2	**(2b)**		**(2a)**		**(2b)**	
z	0.25	0.25	0.2297(37)	0.2448(61)	0.25	0.25
Fe3	**($4f_{IV}$)**		**(2b)**		**($4f_{IV}$)**	
z	0.0256(9)	0.0278(6)	0.0102(41)	0.02516(544)	0.0261(9)	0.0258(6)
Fe33 (2b)						
z	--	--	0.4658(32)	0.4658(63)	--	--
Fe4	**($4f_{VI}$)**		**(2b)**		**($4f_{VI}$)**	
z	0.1917(8)	0.1897(5)	0.1842(32)	0.1846(46)	0.1915(7)	0.1893(4)
Fe44(2b)						
z	--	--	0.2967(35)	0.3046(45)	--	--
Fe5	**(12k)**		**(6c)**		**(12i)**	
x	0.1703(34)	0.1775(26)	0.1606(72)	0.1737(64)	0.1522(41)	0.1814(86)
y	--	--	--	--	0.3435(34)	0.3559(21)
z	-0.1072(4)	-0.1082(3)	0.8785(35)	0.8825(43)	-0.1072(4)	-0.1079(3)
Fe55 (6c)						
x	--	--	0.1763(42)	0.1853(43)	--	--
z	--	--	0.5955(38)	0.5999(41)	--	--
O1	**(4e)**		**(2a)**		**(4e)**	
z	0.1592(16)	0.1548(11)	0.1472(42)	0.1498(39)	0.1603(16)	0.1544(9)
O11 (2a)						
z	--	--	0.3367(53)	0.3479(50)	--	--
O2	**(4f)**		**(2b)**		**(4f)**	
z	- 0.0618(16)	- 0.0569(11)	0.9099(48)	0.9321(57)	-0.0608(16)	-0.0572(10)
O22 (2b)						
z	--	--	0.5327	0.5327(65)	--	--
O3	**(6h)**		**(6c)**		**(6h)**	
x	0.1474(52)	0.1426(37)	0.1413(57)	0.1544(93)	0.1539(54)	0.1436(31)
z	0.25	0.25	0.2519(36)	0.2529(41)	0.25	0.25
O4	**(12k)**		**(6c)**		**(12i)**	
x	0.1527(44)	0.1538(28)	0.1526(68)	0.1592(118)	0.1534(75)	0.1499
y	--	--	--	--	0.3048(41)	0.3123(27)
z	0.0514(6)	0.0524(4)	0.0422(38)	0.0484(36)	0.0523(6)	0.0519(4)
O44 (6c)						
x	--	--	0.1477	0.1476(103)	--	--
z	--	--	0.4397(34)	0.4406(44)	--	--
O5	**(12k)**		**(6c)**		**(12i)**	
x	0.5149(42)	0.5163(30)	0.5269(65)	0.5319(79)	0.5005	0.5217(192)
y	--	--	--	--	1.0258(38)	1.0377
z	0.1490(7)	0.1513(5)	0.1523(45)	0.1520(38)	0.14930(74)	0.1505(5)
O55 (6c)						
x	--	--	0.4990(99)	0.4853(102)	--	--
z	--	--	0.3467(35)	0.3454(45)	--	--
R_{wp}, %	9.98	7.01	8.64	6.92	9.43	7.26
R_{exp}, %	3.83	3.98	3.81	3.95	3.82	3.99
R_B, %	9.34	2.74	4.91	2.29	8.25	3.95
R_{Mag}, %	3.90	1.47	3.03	1.29	2.35	2.89
χ^2	6.80	3.10	5.15	3.06	6.09	3.31