Crystal, magnetic, and electronic structures, and properties of new BaMn*Pn*F (*Pn* = As, Sb, Bi)

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Supporting Information

Table S1 Rietveld refinement results of room temperature powder X-ray diffraction data for BaMnAsF, BaMnSbF and BaMnBiF, with *P*4/*nmm*.

Atom	Wyckoff site	*x*	*y*	*z*	U_{eq} (Å^2)
		BaMnAsF			
		a = 4.2739(1) Å, *c* = 9.5875(2) Å			
Ba	2*c*	0.25	0.25	0.3419(3)	0.026(1)
Mn	2*a*	0.25	0.75	0	0.018(3)
As	2*c*	0.25	0.25	0.8447(5)	0.010(2)
F	2*b*	0.25	0.75	0.5	0.014(7)
		BaMnSbF			
		a = 4.4791(1) Å, *c* = 9.8297(2) Å			
Ba	2*c*	0.25	0.25	0.3541(2)	0.024(2)
Mn	2*a*	0.25	0.75	0	0.022(3)
Sb	2*c*	0.25	0.25	0.8321(2)	0.021(2)
F	2*b*	0.25	0.75	0.5	0.029(8)
		BaMnBiF			
		a = 4.5384(1) Å, *c* = 9.8929(2) Å			
Ba	2*c*	0.25	0.25	0.3578(2)	0.018(1)
Mn	2*a*	0.25	0.75	0	0.030(2)
Bi	2*c*	0.25	0.25	0.8244(2)	0.024(1)
F	2*b*	0.25	0.75	0.5	0.017(6)

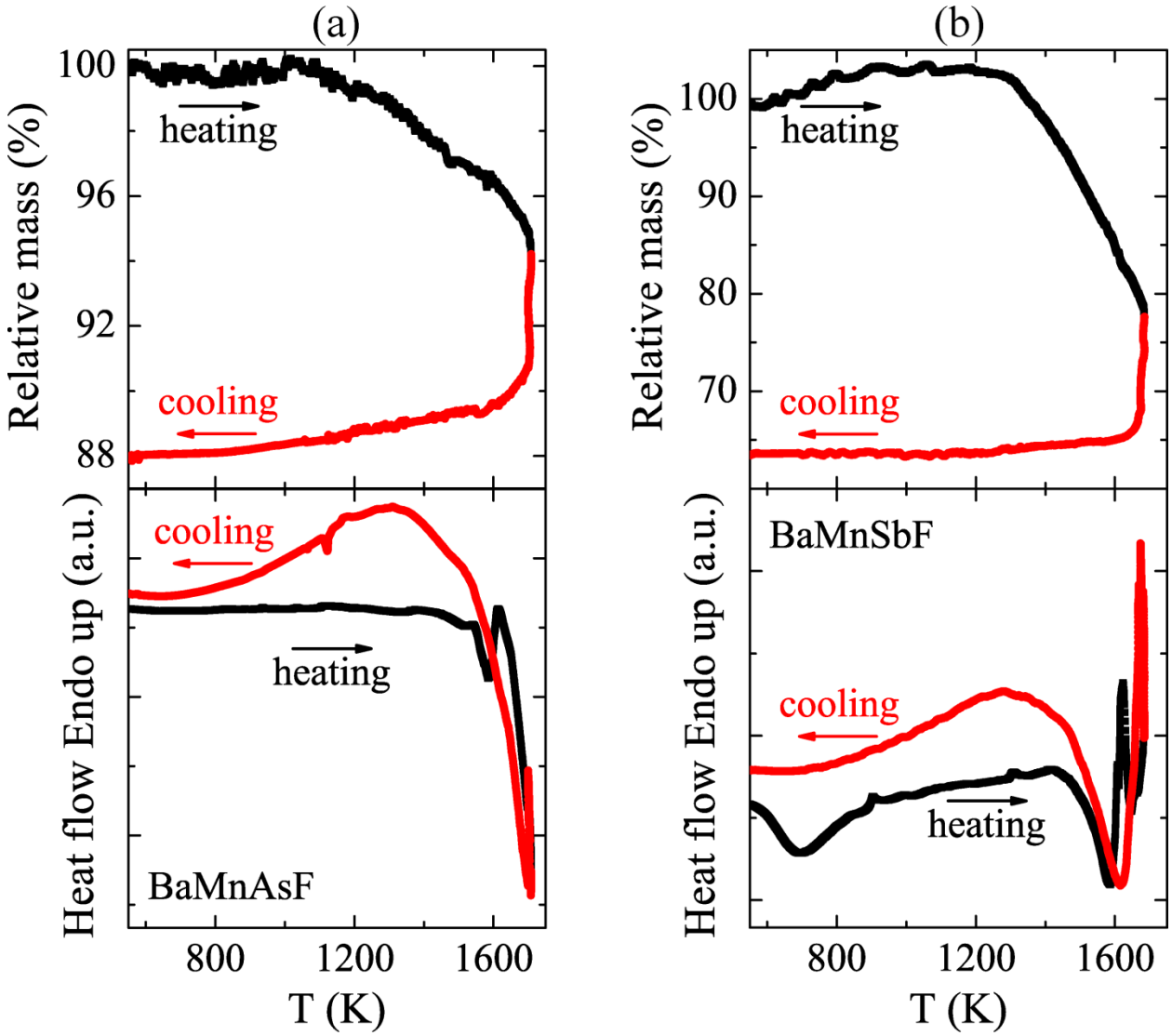

Figure S1. TGA and DTA data for (a) BaMnAsF and (b) BaMnSbF.

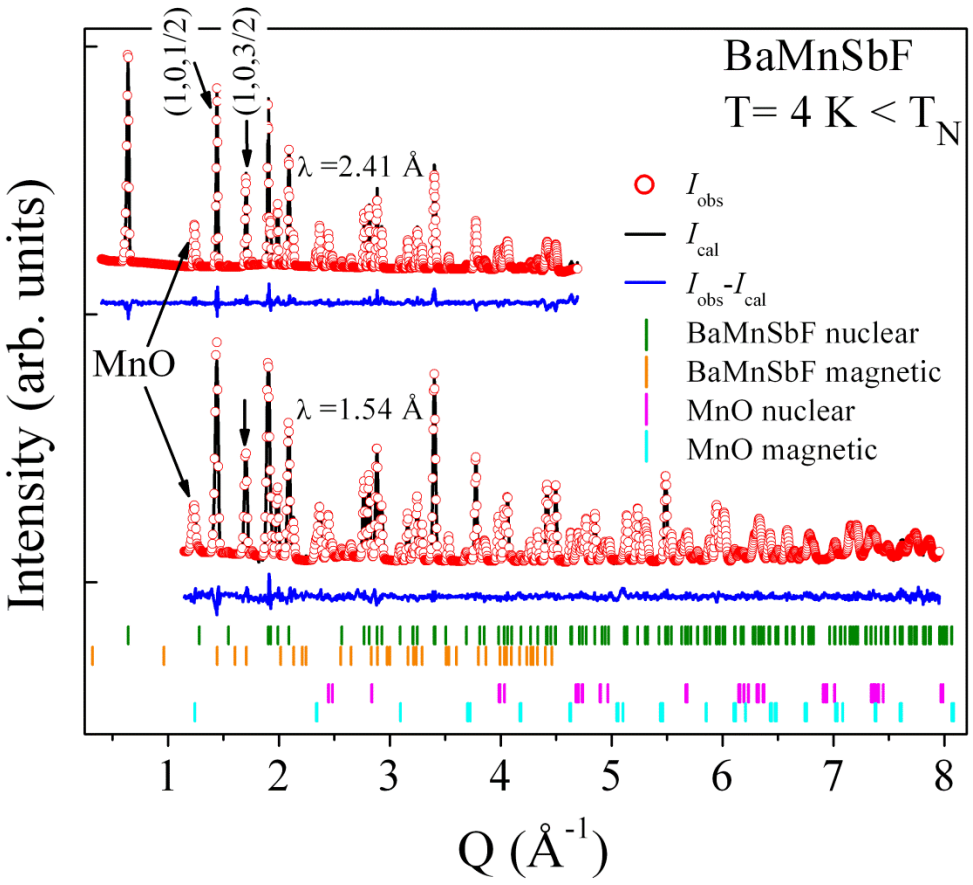

Figure S2. Rietveld plots of the NPD data for BaMnSbF collected at 4 K using 1.54 Å and 2.41 Å wavelengths. The two most prominent magnetic reflections, indexed as (1 0 1/2) and (1 0 3/2), are indicated by arrows. Contribution to patterns in weight fraction are BaMnSbF: 95.2(1.7)%; BaF_2: 2.46(0.03)%; $Mn_{1-x}O$: 2.4(0.2)%. Note: the MnO is monoclinic at low temperatures. Structural distortion is shown to appear in the non-stoichiometric MnO.

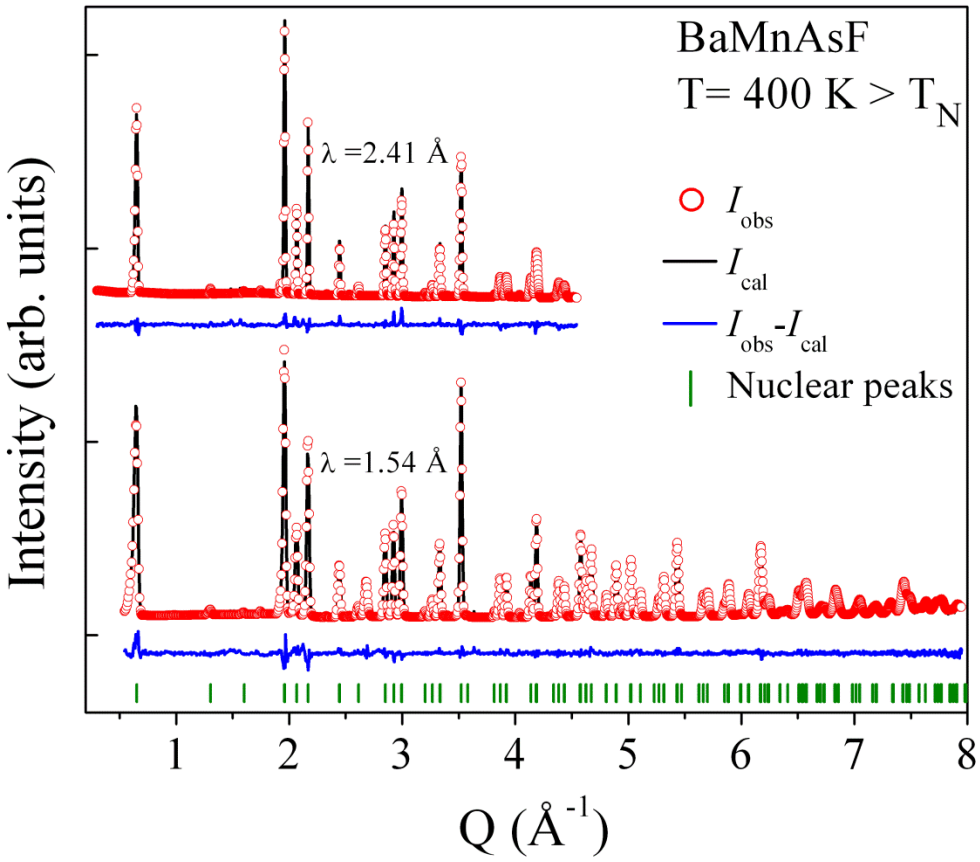

Figure S3. Rietveld plots of the NPD data for BaMnAsF collected at 400 K using 1.54 Å and 2.41 Å wavelengths. Only nuclear Bragg peaks are observed.

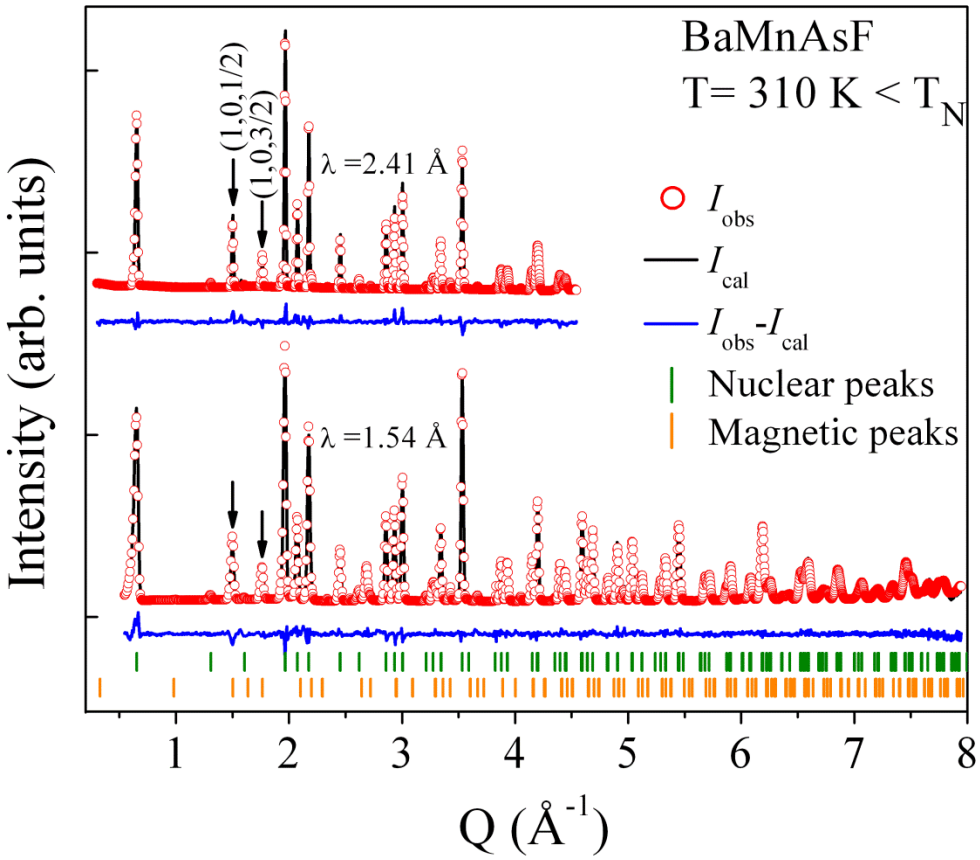

Figure S4. Rietveld plots of the NPD data for BaMnAsF collected at 310 K using 1.54 Å and 2.41 Å wavelengths. The two most prominent magnetic reflections, indexed as (1 0 1/2) and (1 0 3/2), are marked by arrows.

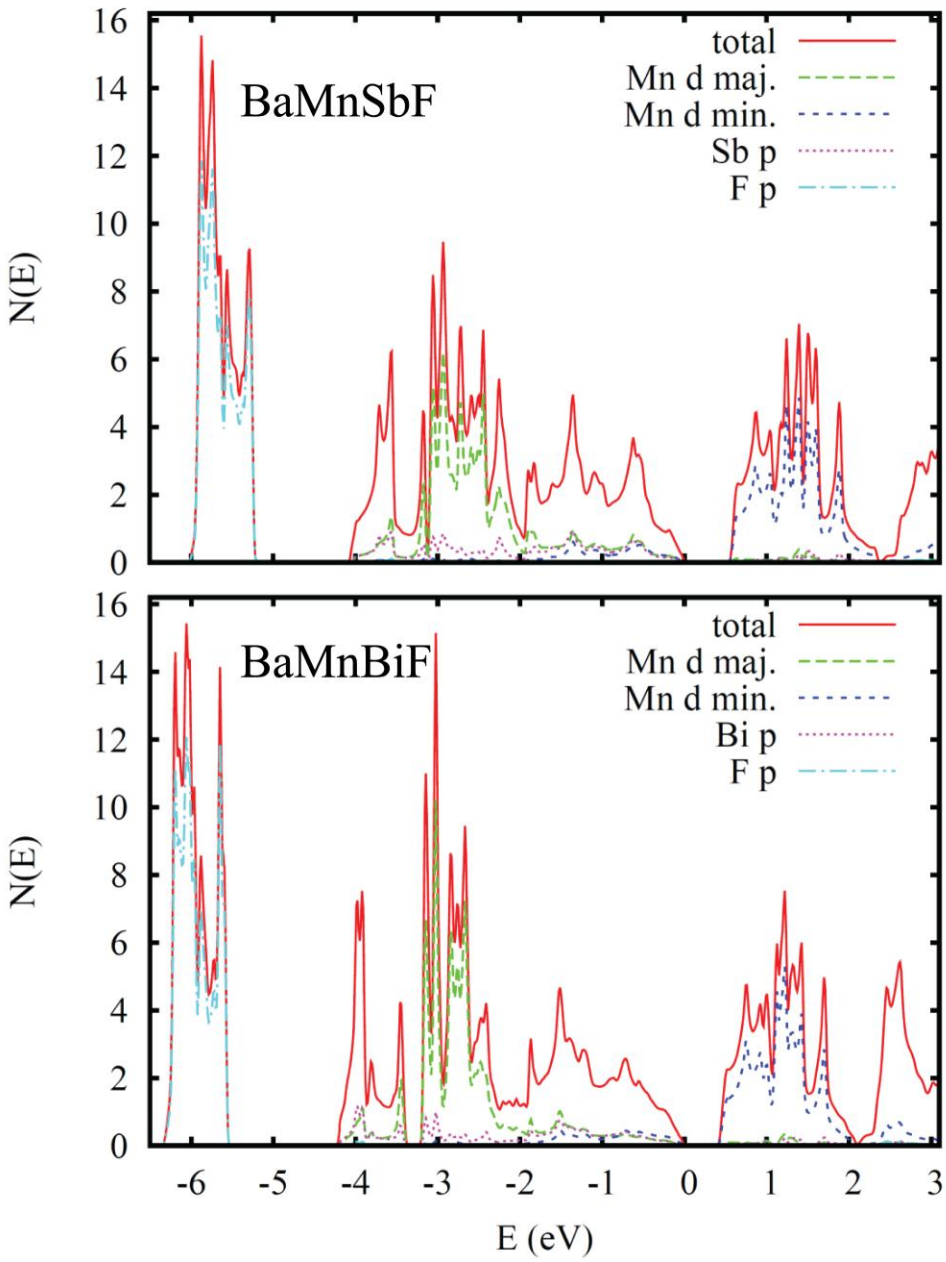

Figure S5. Electronic DOS and projections for BaMnSbF and BaMnBiF in the nearest neighbor in plane antiferromagnetic state. The DOS are per formula unit, both spins and the energy zero is at the valence band maximum.

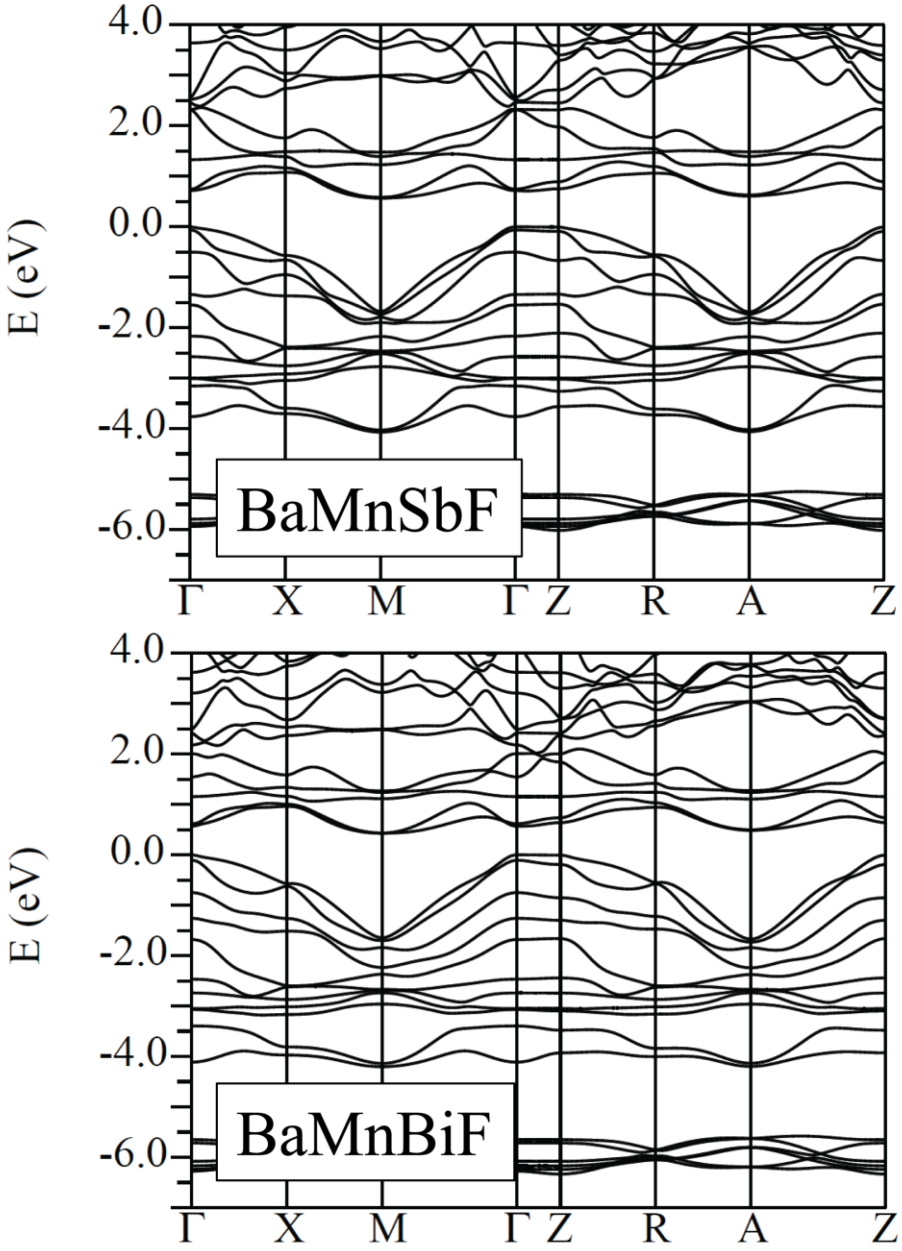

Figure S6. Band structures for BaMnSbF and BaMnBiF in the nearest neighbor in plane antiferromagnetic state. The energy zero is set to the valence band maximum.