Supplementary Information for:

The role of exchange-correlation functional on the description of multiferroic properties using Density Functional Theory: The $ATiO_3$ (A = Mn, Fe, Ni) case study

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Table S1: Calculated lattice parameters (Å) and unit cell volume (Å^3) for the $ATiO_3$ (A = Mn, Fe, Ni) materials as obtained from different exchange-correlation functionals. Experimental and DFT+U results are included for comparison.

		LDA	PBESol	PBE0	PBE0+D	B3LYP	B3LYP+D	DFT+U		Experimental
$MnTiO_3$	a	5.120	5.173	5.209	5.203	5.242	5.238	5.245[a]	5.127[b]	5.205[c]
	c	13.499	13.624	13.632	13.452	13.866	13.536	13.985	13.63	13.700
	V	306.434	315.779	320.371	315.394	330.025	320.426	333.18	310.28	321.400
$FeTiO_3$	a	5.009	5.061	5.156	5.148	5.191	5.176	5.050[b]		5.127[d]
	c	13.617	13.734	13.612	13.458	13.801	13.534	13.520		13.723
	V	295.830	304.632	313.394	308.902	322.058	313.952	298.600		312.420
$NiTiO_3$	a	4.936	4.992	5.039	5.030	5.077	5.061	4.985[e]	4.930[b]	5.021[f]
	c	13.569	13.692	13.710	13.564	13.869	13.618	13.778	13.650	13.840
	V	286.295	295.484	301.423	297.210	309.614	302.070	296.550	287.310	302.167

[a] Reference [1].
[b] Reference [2].
[c] Reference [3].
[d] Reference [4].
[e] Reference [5].
[f] Reference [6].

Table S2: Theoretical short and long M-O (M = Mn, Fe, Ni, Ti) bond distances and octahedral distortion (Δ) for $ATiO_3$ (A = Mn, Fe, Ni) materials as function of the exchange-correlation functionals.

		A-O			Ti-O		
		Short	Long	Δ x 10^{-4}	Short	Long	Δ x 10^{-4}
$MnTiO_3$	B3LYP	2.132	2.300	14.369	1.876	2.142	43.827
	B3LYP+D	2.093	2.352	33.951	1.873	2.099	32.374
	PBE0	2.116	2.299	17.181	1.873	2.093	30.771
	PBE0+D	2.095	2.329	27.977	1.870	2.072	26.258
	PBESol	2.072	2.275	21.808	1.884	2.088	26.378
	LDA	2.042	2.243	22.003	1.876	2.065	22.999
	Experimental[a]	2.118	2.289	15.056	1.866	2.110	37.661
$FeTiO_3$	B3LYP	2.103	2.209	6.043	1.873	2.148	46.773
	B3LYP+D	2.062	2.240	17.120	1.864	2.126	43.118
	PBE0	2.087	2.196	6.477	1.866	2.111	37.951
	PBE0+D	2.065	2.212	11.813	1.861	2.099	36.121
	PBESol	2.019	2.150	9.874	1.896	2.084	22.313
	LDA	1.994	2.124	9.966	1.885	2.064	20.546
	Experimental[b]	2.121	2.159	0.788	1.832	2.133	57.630
$NiTiO_3$	B3LYP	2.059	2.120	2.131	1.865	2.150	50.387
	B3LYP+D	2.027	2.123	5.351	1.853	2.135	50.002
	PBE0	2.040	2.102	2.241	1.857	2.119	43.422
	PBE0+D	2.023	2.103	3.759	1.850	2.110	43.108
	PBESol	2.006	2.081	3.368	1.869	2.099	33.598
	LDA	1.976	2.057	4.034	1.860	2.073	29.330
	Experimental[c]	2.052		-	1.945		-

[a] Reference [7].
[b] Reference [8].
[c] Reference [9].

Table S3: Theoretical results for overlap population (in m|e|) of the A-O bonds (A = Mn, Fe, Ni) as function of exchange-correlation functionals.

	short			long		
	Mn	Fe	Ni	Mn	Fe	Ni
B3LYP	-9.0	5.0	8.0	0.0	7.0	9.0
B3LYP+D	-13.0	2.0	6.0	0.0	6.0	9.0
PBE0	-14.0	1.0	6.0	-2.0	4.0	7.0
PBE0+D	-17.0	-1.0	4.0	-2.0	4.0	7.0
PBESol	-10.0	12.0	14.0	2.0	13.0	13.0
LDA	-12.0	11.0	13.0	1.0	12.0	12.0

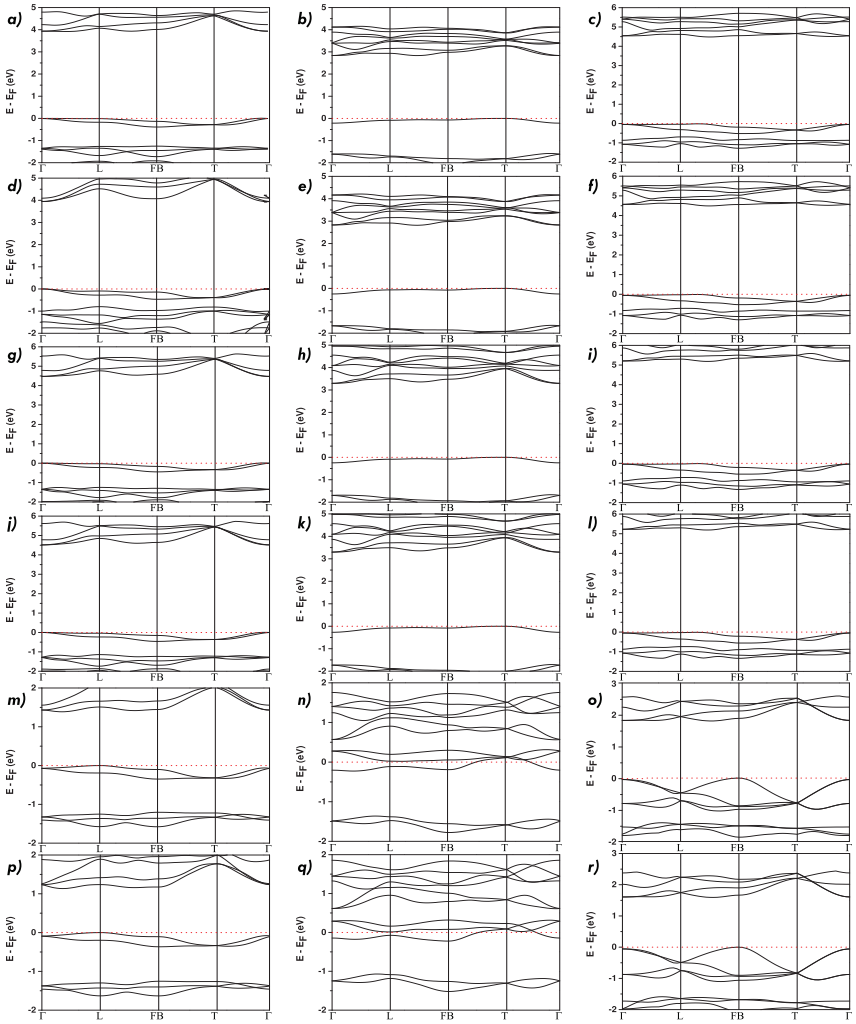

Figure S1: Band Structure profiles for $MnTiO_3$ (left panel), $FeTiO_3$ (middle panel), and $NiTiO_3$ (right panel) materials in G-type antiferromagnetic ground-state obtained from different exchange-correlation functionals. (a-c) B3LYP, (d-f) B3LYP+D, (g-i) PBE0, (j-l) PBE0+D, (m-o) PBESol, (p-r) LDA. In all cases the Fermi level was set to zero.

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