Electronic Supplementary Material (ESI) for RSC Advances.

Table 1

Work of separation Wsep in J/m^2 and bond lengths in Å for left and right interfaces of the $Fe_4N/BaTiO_3$ and $MnFe_3N/BiFeO_3$ interfaces.

	$Fe_4N/BaTiO_3$				$MnFe_3N/BiFeO_3$					
Interface	FeN/TiO_2		Fe_2/TiO_2		FeN/TiO_2		$MnFe/TiO_2$		Mn_2/TiO_2	
	Left	Right	Left	Right	Left	Right	Left	Right	Left	Right
Fe^{I}-O	-	-	2.006	2.010	-	-	-	-	-	-
Fe^{II}-O	2.066	2.264	1.879	1.898	2.040	2.143	1.900	1.924	-	-
N-Ti	2.186	1.954	-	-	2.226	1.981	-	-	-	-
Fe^{I}-Ti	-	-	2.987	2.745	-	-	-	-	-	-
Fe^{II}-Ti	3.008	2.848	2.867	2.638	2.973	2.760	2.995	2.732	-	-
Mn^{I}-O	-	-	-	-	-	-	2.039	2.045	2.066	2.092
Mn^{II}-O	-	-	-	-	-	-	-	-	1.963	1.985
Mn^{I}-Ti	-	-	-	-	-	-	2.969	2.765	3.06	2.905
Mn^{II}-Ti	-	-	-	-	-	-	-	-	3.013	2.849
Wsep	2.075		3.263		2.222		4.162		2.547	

Table 2

Magnetic moments (in μ_B) of the interfacial atoms in the $Fe_4N/BaTiO_3$ junction. The $\Delta\mu(\text{left}-\text{right})$ is the difference between the magnetic moments at the right and left interfaces.

Interface	Atom	Middle	Left	Right	$\Delta\mu(\text{left}-\text{right})$
FeN/TiO_2	Fe^{II}	5.075	5.467	5.362	0.105
	N	0.025	0.027	0.019	0.008
	Ti	0.000	-0.005	-0.06	0.055
	O^{I}	0.000	0.048	0.053	-0.005
	O^{II}	0.000	0.063	0.043	0.020
	Fe^{III}	2.527	2.125	2.383	-0.258
	Fe^{IV}	3.009	2.978	2.968	0.01
Fe_2/TiO_2	Fe^{I}	3.003	2.995	2.884	0.111
	Fe^{II}	2.347	2.580	2.285	0.295
	Ti	0.000	-0.068	-0.45	0.382
	O^{I}	0.000	0.038	0.043	-0.005
	O^{II}	0.000	0.055	0.047	0.008
	Fe^{III}	2.505	2.454	2.447	0.008
	Fe^{IV}	2.517	2.454	2.427	0.027
	N	0.027	0.017	0.009	0.008

Table 3

Magnetic moments (in μ_B) of the interfacial atoms in the $MnFe_3N/BaTiO_3$ junction. The meanings of $\Delta\mu(\text{left}-\text{right})$ is the same as Table 2.

Interface	Atom	μ(Middle)	$\mu(I_L)$	$\mu(I_R)$	$\Delta\mu(I_L - I_R)$
FeN/TiO_2	Fe^{II}	4.894	5.412	5.264	0.148
	N	0.018	0.038	0.027	0.011
	Ti	0.000	-0.024	-0.104	0.080
	O^{I}	0.000	0.056	0.061	-0.005
	O^{II}	0.000	0.068	0.053	0.015
	Fe^{III}	2.397	2.181	2.384	-0.203
	Mn	3.960	3.963	3.968	-0.005
$MnFe/TiO_2$	Mn^{I}	3.956	4.029	3.882	0.147
	Fe^{II}	2.348	2.510	2.285	0.225
	Ti	0.000	-0.052	-0.513	0.461
	O^{I}	0.006	0.010	0.024	-0.014
	O^{II}	0.000	0.064	0.059	0.005
	Fe^{III}	2.409	2.447	2.408	0.039
	Fe^{IV}	2.422	2.471	2.452	0.019
	N	0.019	0.023	0.013	0.01
Mn_2/TiO_2	Mn^{I}	3.954	3.984	3.904	0.08
	Mn^{II}	-	3.681	3.559	0.122
	Ti	0.000	-0.009	-0.447	0.438
	O^{I}	0.000	0.016	0.033	-0.017
	O^{II}	0.000	0.017	0.027	-0.01
	Fe^{III}	2.408	2.415	2.383	0.032
	Fe^{IV}	2.421	2.424	2.425	-0.001
	N	0.02	-0.007	-0.013	0.006