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Supplemental Material

Orbital Controlled Band Gap Engineering of Tetragonal $BiFeO_3$

for Optoelectronic Applications

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Table 1. Average atomic magnetic moment (MM) for Fe and TM (TM=Cr, Mn and Co) and total magnetic moment for $BiFe_{1-x}TM_xO_3$.

$BiFe_{1-x}TM_xO_3$	TM=Cr			TM=Mn			TM=Co		
MM (μB)	Fe	Cr	Total	Fe	Mn	Total	Fe	Co	Total
x=0.0	4.136	0	0	4.136	0	0	4.136	0	0
x=0.125	4.1376	2.884	-1.909	4.137	3.770	-0.975	4.134	2.986	-0.995
x=0.25	4.142	2.886	0	4.140	3.771	0	4.133	2.980	0
x=0.375	4.147	2.891	1.932	4.139	3.781	0.98	4.132	2.978	0.995
x=0.5	4.152	2.894	0	4.137	3.787	0	4.134	2.975	0
x=0.625	4.164	2.901	-1.932	4.142	3.777	-0.975	4.130	2.976	-0.996
x=0.75	4.190	2.911	0	4.175	3.920	32.899	4.128	2.975	0
x=0.875	4.222	2.932	-1.965	4.185	3.916	31.935	4.125	2.974	-0.996
x=1.0	0	2.944	0	0	3.908	30.963	0	2.972	0

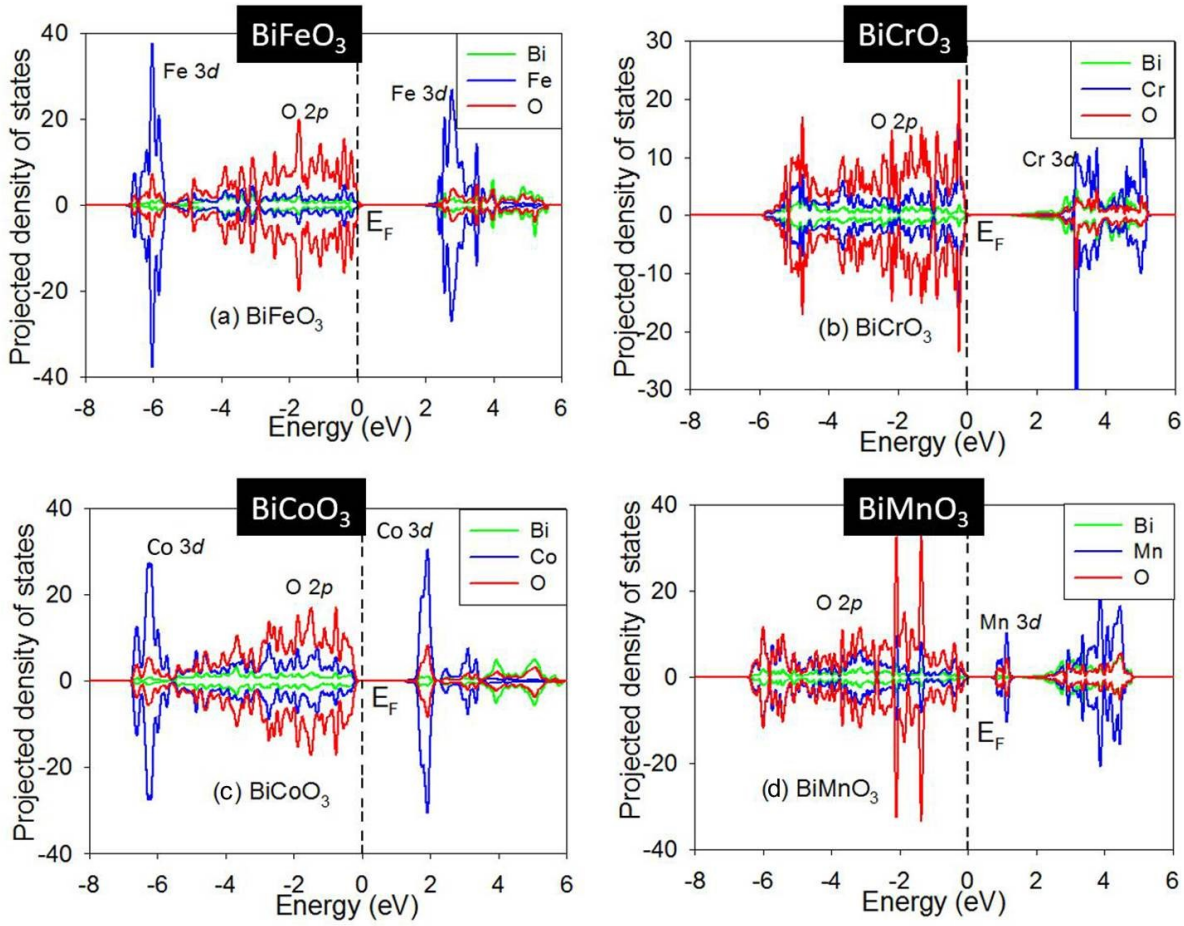

Fig. S1 Calculated density of states for matrix materials.

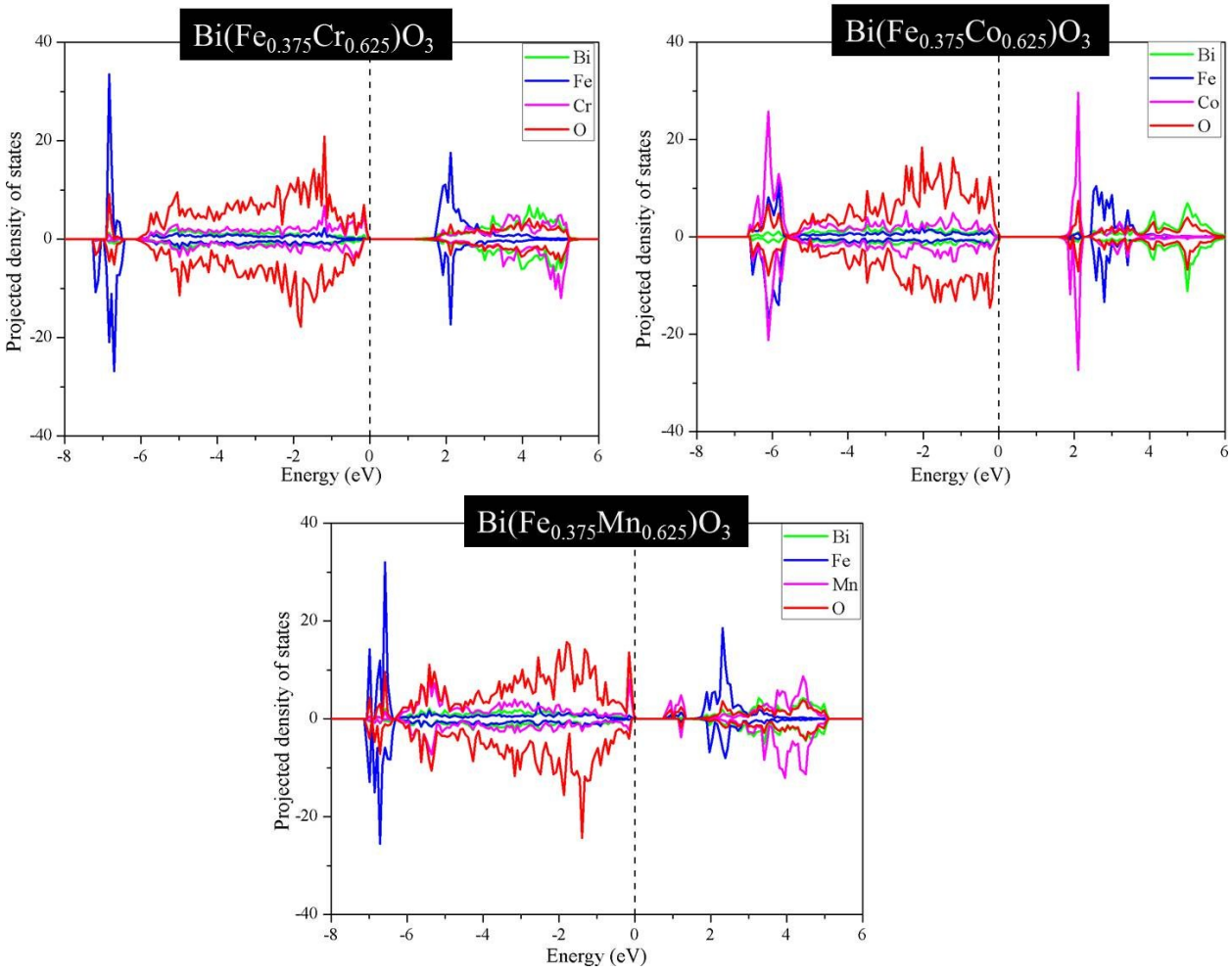

Fig. S2 Calculated density of states for Cr-, Mn-, and Co- doped $BiFeO_3$.