

1 **ADFT investigation of the role of oxygen vacancies on the structural, electronic and magnetic properties**  
2 **of ATiO<sub>3</sub> (A = Mn, Fe, Ni) multiferroic materials**

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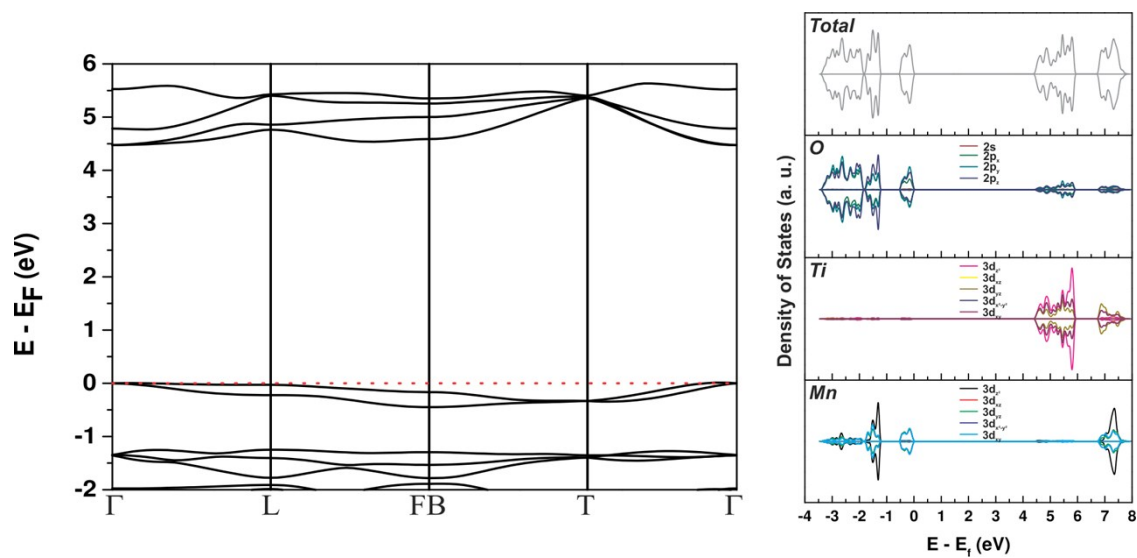
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10 ***SUPPORTING INFORMATION***

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12 **Figures**

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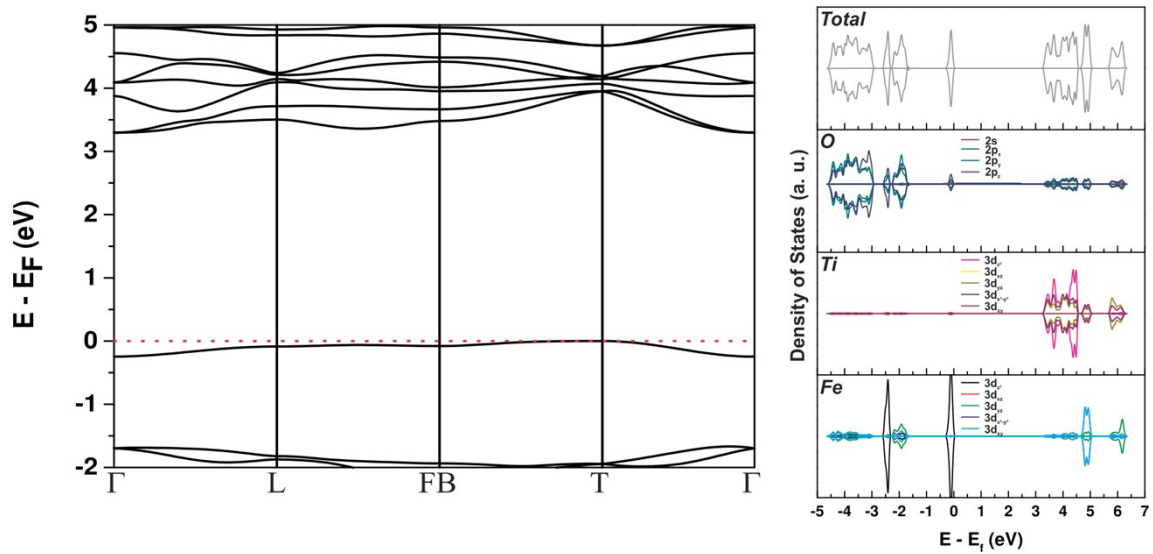
15 **Figure S1.** Band structure profile (left panel) and orbital resolved DOS (right panel) for pristine  $\text{MnTiO}_3$ . The

16 Fermi level was set as zero in all cases.

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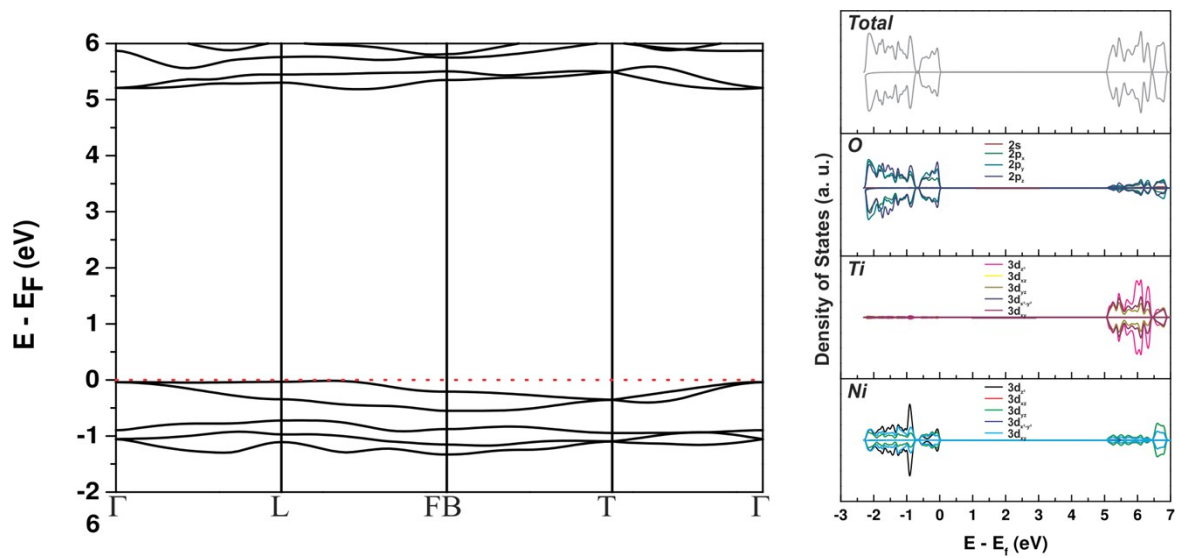


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21 **Figure S2.** Band structure profile (left panel) and orbital resolved DOS (right panel) for pristine FeTiO<sub>3</sub>. The  
 22 Fermi level was set as zero in all cases.

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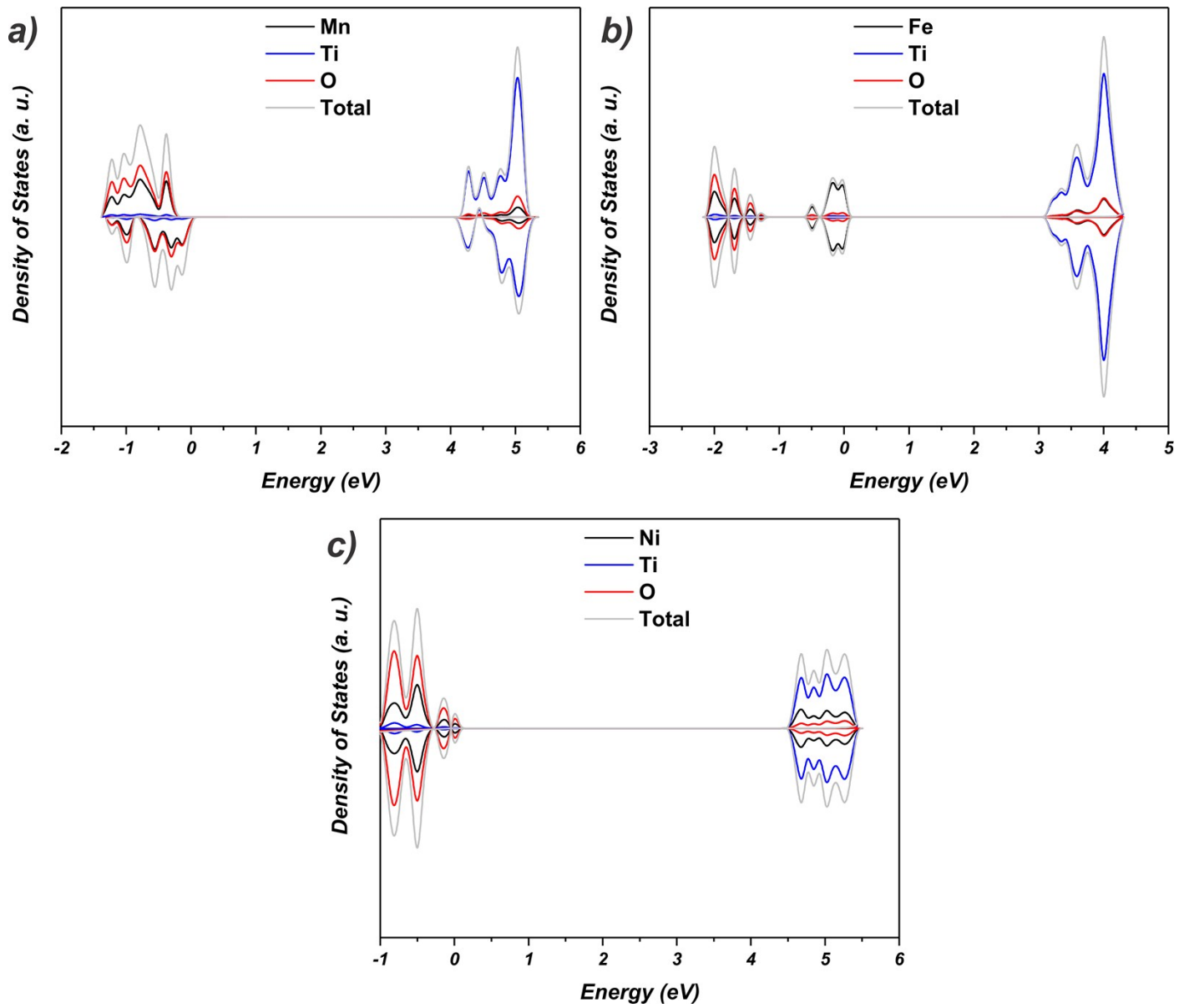


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26 **Figure S3.** Band structure profile (left panel) and orbital resolved DOS (right panel) for pristine NiTiO<sub>3</sub>. The

27 Fermi level was set as zero in all cases.

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30 **Figure S3.** DOS profiles for pristine a) MnTiO<sub>3</sub>, b) FeTiO<sub>3</sub> and c) NiTiO<sub>3</sub>. The Fermi level was set as zero in  
 31 all cases.

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