

**Supplementary Material for “First-principles study the electric, magnetic, and orbital structure in perovskite  $\text{ScMnO}_3$ ”**

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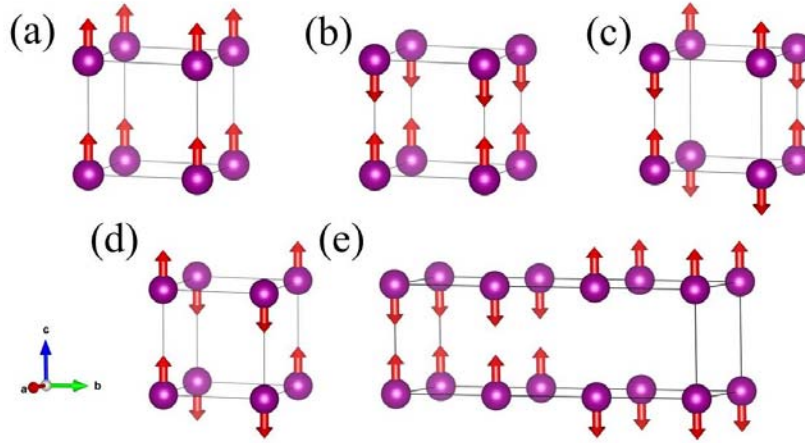


Figure. S1. The schematic diagram of ferromagnetic (FM) (a), A-AFM (b), C-AFM (c), G-AFM (d), and E-AFM (e) magnetic ordering calculated in the main text. The Sc and O atoms are not shown in this schematic. The A-AFM shows ferromagnetic (antiferromagnetic) intraplanar (interplanar) coupling; the C-AFM shows ferromagnetic (antiferromagnetic) interplanar (intraplanar) coupling; the G-AFM shows AFM in both intra- and interplanar coupling. The E-AFM shows in-plane FM zigzag chains antiferromagnetically coupled to the neighboring chains; the interplanar coupling is also AFM.

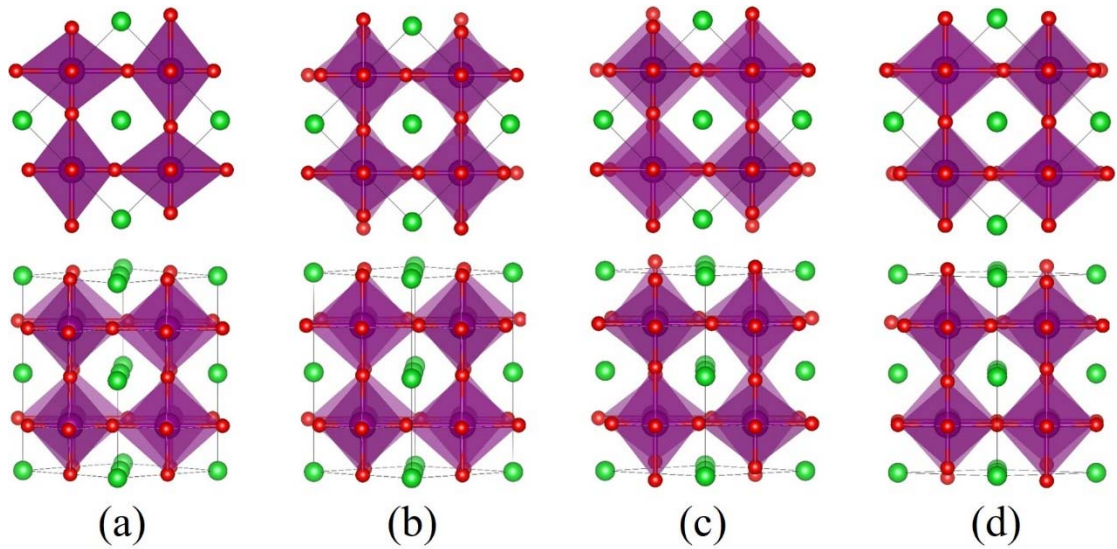


Figure. S2. The schematic diagram of different distortions of  $\text{MnO}_6$  octahedral. The first layer represents polyhedral views of these phases from the  $z$ -axis, while the second layer is the view from the  $x$  and  $y$ -axes. In the schematic diagram the tilt and rotation of  $\text{MnO}_6$  octahedral are not shown. (a)  $\text{LaMnO}_3$ . (b)  $\text{YVO}_3$ . (c) Strained  $\text{LaMnO}_3$ . (d)  $\text{ScMnO}_3$ .