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$\alpha$ -SrMnO<sub>3</sub>

## First-Principles Study on the Electronic Structures of $\alpha$ -SrMnO<sub>3</sub>

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The electronic structures of hexagonal  $\alpha$ -SrMnO<sub>3</sub> were studied by first-principles calculations within plane wave pseudopotential method. The calculated results indicate that the  $\alpha$ -SrMnO<sub>3</sub> is antiferromagnetic

moment of the Mn<sup>4+</sup>. The spin exchange coupling constants are fit within the Noodleman's broken symmetry methods through the calculated total energy for the various spin ordered states of  $\alpha$ -SrMnO<sub>3</sub>. The local microstructures(Mn—O—Mn) of  $\alpha$ -SrMnO<sub>3</sub> determine the special magnetic exchange interaction. There are AFM exchange interactions both within the Mn<sub>2</sub>O<sub>9</sub> entities and between the Mn ions in the corner-sharing octahedron of  $\alpha$ -SrMnO<sub>3</sub>, and the latter AFM exchange interaction is stronger than the former one.

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