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Magnetic properties of the double perovskite $\text{Sr}_2\text{FeOsO}_6$: microscopic insights from ab-initio density-functional theory study SUDIPTA KANUNGO, BINGHAI YAN, Max Plack Institute for Chemical Physics of Solids, MARTIN JANSEN, Max Plack Institute for Solid State Research, CLAUDIA FELSER, Max Plack Institute for Chemical Physics of Solids — Using density-functional theory calculations, we investigated the electronic and magnetic properties of the ordered 3d-5d double perovskite $\text{Sr}_2\text{FeOsO}_6$, which has recently drawn attention for interesting antiferromagnetic (AFM) phase transitions in low temperature observed in experiments. The calculated effective magnetic exchange interactions reveal the importance of long-range super-superexchange interactions in this compound. The competition between the ferromagnetic (FM) Os-O-Fe short-range interaction and AFM Os-O-Fe-O-Os long-range interaction induces strong magnetic frustration along the crystallographic c axis. This strong magnetic frustration is proposed to drive the magnetic phase transition between two AFM phases (AFM1 to AFM2) and related lattice distortion, which were also observed in the experiment. [Ref: Sudipta Kanungo, Binghai Yan, Martin Jansen, and Claudia Felser; Phys. Rev. B 89, 214414 (2014)]

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