Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

On the magnetic structure and band gap of the double perovskite Ba2CuOsO6: Density functional analysis[1] CHANGHOON LEE, JISOOK HONG, JI HOON SHIM, Pohang University of Science and Technology, MYUNG-HWAN WHANGBO, North Carolina State University — The ordered double-perovskite Ba_2CuOsO_6, consisting of 3d and 5d transition-metal magnetic ions (Cu^{2+} and Os^{6+}, respectively), is a magnetic insulator. It obeys the Curie-Weiss law with θ = -13.3 K. We evaluated the spin exchange interactions of Ba_2CuOsO_6 by performing energy-mapping analysis based on DFT+U calculations and determined the band gap of Ba_2CuOsO_6 by DFT+U and DFT+U+SOC calculations. The antiferromagnetic ordering of Ba_2CuOsO_6 is due largely to the spin exchange interactions between Cu2+ ions, which are enhanced by the empty eg orbitals of the intervening Os^{6+} ions. Both electron correlation and spin-orbit coupling are necessary to open a band gap for Ba_2CuOsO_6.

[1]2013R1A1A2060341

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Date submitted: 05 Nov 2015 Electronic form version 1.4