A tale of three double perovskites: $\text{Ba}_2\text{XOsO}_6$ ($\text{X}=\text{Na, Ca, Y}$)\(^1\)

SHRUBA GANGOPADHYAY, WARREN PICKETT, University of California - Davis — High valent Os based double perovskites are one center of current interest because they display extreme interplay of large spin orbit coupling and strong electronic correlation. We present electronic and magnetic structures of three cubic Os based double perovskites with Os\(^{7+}\) ($d^1$), Os\(^{6+}\)($d^2$), Os\(^{5+}\)($d^3$). For these first principles based calculation we used an onsite hybrid exchange only on Os(5d), as implemented in Wien2k. While $\text{Ba}_2\text{NaOsO}_6$ is a ferromagnetic Mott insulator, the other two show antiferromagnetic ordering. For comparison purposes we have investigated only the ferromagnetic ordered phase of these three materials. A metal-insulator transition by changing spin orbit coupling direction is found in all three materials, however each double perovskite is metallic for different magnetic directions. Surprises from looking at the radial charge densities will be discussed. We provide a resolution to the riddle: why, despite d1 configuration, does $\text{Ba}_2\text{NaOsO}_6$ remain cubic. This material introduces a new class of J= 3/2 Mott insulator.

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