A tale of three cubic double perovskites: Ba_2XOsO_6, X=Na, Ca, Y

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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} $(d^1), Os^{+6}(d^2), Os^{+5}(d^3)$. Despite of d^1 and d^2 configuration Ba_2NaOsO_6 shows very little Jahn-Teller distortion, and Ba_2CaOsO_6 also remains cubic. For these first principles based calculation we used an onsite hybrid exchange only on Os(5d), as implemented in Wien2k. While Ba_2NaOsO_6 is a ferromagnetic Mott insulator, the other two show antiferromagnetic ordering. Our approach faithfully reproduce experimental magnetic moments and Mott insulating state for these perovskites.[1] 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 observed in all three materials, however each double perovskite is metallic for different magnetic directions. In addition to that we are presenting isotropic chemical shielding constants and magnetic susceptibilities for all these three prevoskites with respect to different spin orbit coupling directions, Os shows the most perturbation with change of spin orbit coupling directions. Surprises from looking at the radial charge densities will be discussed.

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[1] S. Gangopadhyay and W. E. Pickett, Physical Review B **91**, 045133 (2015).