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A new bonding insight on Ba_2NaOsO_6 based on orbital-quenching-induced magnetism SHRUBA GANGOPADHYAY, Postdoctoral Associate, Department of Physics, University of California, Davis, KWAN-WOO LEE, Assistant Professor, Department of Applied Physics, Korea University, KYO-HOON AHN, Department of Applied Physics, Korea University, WARREN PICKETT, Distinguished Professor, Department of Physics, University of California Davis —
Double perovskite Ba_2NaOsO_6 (BNOO) is an exotic example of a heptavalent osmium compound, and also uncommon by being a ferromagnetic insulator. Although the single 5d t_{2g} electron from Os orders magnetically, there is no evidence of orbital order that would destroy its cubic symmetry. Local density approximation with Hubbard U (LDA+U) calculation revealed very strong Os d – O p hybridization into weakly overlapping cluster orbitals, but was unable to obtain the observed Mott insulating behavior. The gap can obtained using DFT+U+ spin-orbit coupling (SOC) with unreasonably high value of U. Building from the basic understanding from LDA+U calculations, we have performed hybrid DFT studies, including SOC, implemented in Wien2k. This method obtains a narrow gap, and an orbital moment of -0.42 muB that strongly compensates the +0.52 muB spin moment. The effects of SOC on the spin density will be presented and discussed, as will the change in the electronic and magnetic properties under pressure.

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