Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

DFT+U study of electronic structure and Curie temperature of A_2BReO$_6$ (A=Sr, Ca and B=Cr, Fe) ALEX LEE, CHRIS MARIANETTI, Applied Physics and Applied Math, Columbia University — Re-based double perovskites (DPs) have attracted much attention due to their high Curie temperature (T_C) and colossal magneto resistance with large potential for spintronic applications. Here we investigate the electronic and magnetic properties of the Re-based DPs A_2BReO$_6$ (A=Sr, Ca and B=Cr, Fe) using density functional theory + U (DFT+U) calculations. While monoclinic Ca_2CrReO_6 and Ca_2FeReO_6 (monoclinic) are insulating within GGA+U, tetragonal Sr_2CrReO_6 ($a^0a^0c^0$) and Sr_2FeReO_6 ($a^0a^0c^-$) remain metallic. We show that both on-site interaction U and octahedral tilting are critical to obtain the insulating phases. The $a^0a^0c^-$-phase of Sr_2CrReO_6 is most stable and insulating with nonzero U, suggesting that the high quality Sr_2CrReO_6 film on STO substrate can be a semiconductor as reported in recent experiments. We explain that the insulator-to-metal transition (MIT) of Ca_2FeReO_6 at 140K is predominantly due to a structural phase transition which drives the insulating state. Curie temperatures of Re-based DPs are calculated using the classical Monte Carlo simulations based on the Heisenberg model.

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Date submitted: 06 Nov 2015 Electronic form version 1.4