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**Orbital ordering induced metal-insulator transition in rhenium based double perovskites**<sup>1</sup> ALEX LEE, CHRIS MARIANETTI, Columbia University — Double perovskites (DPs), which are transition metal oxides with two types of transition metals, offer a huge phase space of possibilities and the potential for novel physics. More specifically, Re-based DPs  $A_2B\text{ReO}_6$  ( $A=\text{Sr,Ca}$  and  $B=\text{Cr,Fe}$ ) show interesting insulator to metal transitions (MIT) as a function of temperature. Here we systematically study the electronic properties and MIT of the Re-based DPs using density functional theory +  $U$  and dynamical mean-field theory (DMFT) calculations. We show that the on-site interaction  $U$  for Re is necessary for obtaining the experimentally observed insulating state in  $\text{Sr}_2\text{CrReO}_6$ ,  $\text{Ca}_2\text{CrReO}_6$ , and  $\text{Ca}_2\text{FeReO}_6$ , primarily via the induction of antiferro orbital ordering on the Re sites. This orbital ordering is enhanced by cooperating with local octahedral distortions and tilting. Our predicted insulating ground state of  $\text{Sr}_2\text{CrReO}_6$  is consistent with recent experiments. The experimentally observed MIT at 140K in  $\text{Ca}_2\text{FeReO}_6$ , is elucidated by using the experimental structures just below and above the phase transition. We find that  $\text{Sr}_2\text{FeReO}_6$  remains metallic, yielding a qualitatively consistent description of this entire family. Specific comparisons will be made between DFT+ $U$  and DFT+DMFT calculations.

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