DFT+$U$ study of electronic structure and Curie temperature of $A_2B\text{ReO}_6$ ($A=$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 $A_2B\text{ReO}_6$ ($A=$Sr, Ca and $B=$Cr, Fe) using density functional theory + $U$ (DFT+$U$) calculations. While monoclinic $\text{Ca}_2\text{CrReO}_6$ and $\text{Ca}_2\text{FeReO}_6$ (monoclinic) are insulating within GGA+$U$, tetragonal $\text{Sr}_2\text{CrReO}_6$ ($a_0a_0c_0^\pi$) and $\text{Sr}_2\text{FeReO}_6$ ($a_0a_0c_0^-$) remain metallic. We show that both on-site interaction $U$ and octahedral tilting are critical to obtain the insulating phases. The $a_0a_0c_0^-$-phase of $\text{Sr}_2\text{CrReO}_6$ is most stable and insulating with nonzero $U$, suggesting that the high quality $\text{Sr}_2\text{CrReO}_6$ film on STO substrate can be a semiconductor as reported in recent experiments. We explain that the insulator-to-metal transition (MIT) of $\text{Ca}_2\text{FeReO}_6$ 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.