Half Metallicity in Trigonal MnPO₄ and CrPO₄ Crystals
BORIS KIEFER, New Mexico State University — The search for half-metallic compounds continues to be an active area even after several decades of intense research. Half-metals are prime candidates with applications as spin injection materials. Yet, the corresponding material set remains comparatively limited. Here we report a new structural template with Mn and Cr in tetrahedral oxygen coordination. The tetrahedral MnO₄ and CrO₄ groups share corners with intermittent PO₄ groups to form a 3d bond topology. All present computations are based on spin-polarized DFT computations at the GGA-PBE level using all-electron like PAW interaction potentials. The preliminary results show a spin-gap in the minority spin channel for both compounds with magnetic moments of 3 \( \mu_B/\text{fu} \) and 4 \( \mu_B/\text{fu} \) for the Cr and Mn compound, respectively. Furthermore, in both compounds the half-metallic state is energetically more favorable as compared to the competing antiferromagnetic state. Therefore, these compounds which are isomorphic to the previously synthesized Fe analog may provide a new structural class of half-metallic compounds.