Abstract Submitted
for the 4CF15 Meeting of
The American Physical Society

Electronic and Magnetic Properties of $TMPO_4$ (TM=Fe, Mn, Cr) BORIS KIEFER, New Mexico State University — Advances in experiment and theory continue to increase our understanding of macroscopic and atomistic structure/property relationships in materials. However, solving the property to structure problem, and hence rational materials design remains challenging at present. Here we report on the use of a few simple rules to design a structural template for a new class of half-metals. In the proposed structure tetrahedral TMO_4 (TM=Fe, Mn, Cr) groups share corners with intermittent PO_4 groups to form a 3d periodic bond topology. All computations are based on spin-polarized Density-Functional-Theory (DFT) computations at the GGA-PBE level using all-electron like PAW interaction potentials. $FePO_4$ is antiferromagnetic consistent with experimental observations. In contrast, the DFT results for TM= Mn and Cr predict half-metallicity: a spin-gap in the minority spin channel and integer magnetic moments of 3 μ_B/fu and 4 μ_B/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. We will also discuss our DFT+U results that allow assessing the reliability of the DFT predictions that $MnPO_4$ and $CrPO_4$ are half-metals.

Boris Kiefer
New Mexico State University

Date submitted: 11 Sep 2015 Electronic form version 1.4