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 $\mu_B$/fu and 4 $\mu_B$/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.