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Half Metallicity in Trigonal MnPO_4 and CrPO_4 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 MnO_4 and CrO_4 groups share corners with intermittent PO_4 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.

Boris Kiefer
New Mexico State University

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