Compensated Half-Metallicity in the Trigonally Distorted Perovskites

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A compensated half-metal (CHM), also called a half-metallic antiferromagnet, has one conducting and the other insulating spin channels, but zero net moment, resulting in no macroscopic magnetic field. Although CHM is a promising candidate for spintronics, no true CHM has been synthesized yet. Since at least two magnetic ions are required in a unit cell, the double perovskites, the Heusler structures, and tetrahedrally coordinated chalcopyrites have been investigated for last 15 years. However, some complicated details such as antisite disorders and spin-orbit coupling prohibit from synthesizing true CHMs.

In this presentation, we will address a new route to search for CHM. Several trigonally distorted perovskites with two transition metals were synthesized at high pressure 6-7 Gpa at high temperature 1200℃ about forty years ago. Through first principles calculation including the on-site Coulomb repulsion U, we investigated $NiCrO_3$ and as-yet-unsynthesized $PdCrO_3$. Consistent with experimental observations by Chamberland and Claud, $NiCrO_3$ leads to insulating with a few decades meV and ~3 eV for each spin channel, and showing a zero net moment regardless of strength of U. This strong asymmetric gap suggests a insulator-CHM transition under modest pressure. Futhermore, our calculations of an isovalent and isostructural $PdCrO_3$, which is expected to have less correlation strength, show that $PdCrO_3$ is a true CHM even for ambient pressure. These findings provide another structure class that may be favorable for synthesis of CHM.

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