

Abstract Submitted
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Ferromagnetic ordering and halfmetallic state in a shandite: $\text{Co}_3\text{Sn}_2\text{S}_2$ ¹ HELGE ROSNER, MPI for Chemical Physics of Solids Dresden, RICHARD WEIHRICH, Institute for Inorganic Chemistry, University Regensburg, WALTER SCHNELLE, MPI for Chemical Physics of Solids Dresden — The recent rapid development in spintronics challenges the search for new magnetic half metals with high Curie temperatures as well as an improved understanding of the underlying microscopic properties. Here, we present a joint experimental and theoretical study of the recently reinvestigated shandite $\text{Co}_3\text{Sn}_2\text{S}_2$ [1]. From magnetic susceptibility, specific heat and resistivity measurements on powder samples we find a phase transition to a ferromagnetic metallic state at 177 K with a saturation moment of 0.87 μ_B /f.u. Full potential electronic structure calculations within the local spin density approximation result in a halfmetallic ferromagnetic groundstate with a moment of 1 μ_B /f.u. and a tiny gap in the minority spin channel. The calculated structure optimization and structure variations show that the size of the gap is rather sensitive to the lattice geometry. Possibilities to stabilize the halfmetallic ferromagnetic behaviour by various substitutions have been studied theoretically and will be discussed in detail.

[1]R. Wehrich *et. al.* Z. Anorg. Allg. Chem. **630**, 1767, (2004)

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