

Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Ferromagnetic ordering and halfmetallic state in a shandite:
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The rapid advance in spintronics challenges an improved understanding of the under-
lying microscopic properties. Here, we present a joint experimental and theoretical
study of Co₃Sn₂S₂ (shandite) and related compounds. From magnetic susceptibil-
ity, specific heat and magneto-transport measurements on a shandite single crystal
sample we find a phase transition to a ferromagnetic metallic state at 177 K with a
saturation moment of 0.92 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 chan-
nel. 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 behavior by various substitutions have been studied
theoretically and will be discussed.

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Date submitted: 09 Nov 2012

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