

Abstract Submitted  
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**Electronic and thermoelectric properties of CoSbS and FeSbS<sup>1</sup>**

DAVID PARKER, Oak Ridge National Laboratory, ANDREW F. MAY, HSIN WANG, MICHAEL A. MCGUIRE, BRIAN C. SALES, DAVID J. SINGH, ORNL — We present a combined theoretical and experimental study of the potential thermoelectric performance of three transition metal antimonide sulfides, CoSbS, FeSbS and NiSbS. From theory we find that NiSbS is metallic and hence of little interest regarding thermoelectric performance. CoSbS and FeSbS are both semiconductors with rather heavy valence and conduction bands, whose thermopower can exceed  $200 \mu\text{V}/\text{K}$  at temperatures of 900 K and carrier concentrations of  $10^{21}\text{cm}^{-3}$ , which is similar to the *n*-type high performance thermoelectric filled skutterudites. The experimental results on several non-optimized *n*-type CoSbS samples confirm its semiconducting nature and indicate a potential for good high temperature thermoelectric performance, finding a *ZT* for two of the samples of 0.35 at 773 K. Substantially higher *ZT* values may be possible if the lattice thermal conductivity can be reduced by alloying and the effects of extrinsic scattering, which appear to be substantial in the experimental results, are reduced.

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