

Abstract Submitted  
for the MAR10 Meeting of  
The American Physical Society

**Validity of Wiedemann-Franz law in thermoelectric half Heusler compounds**<sup>1</sup> MAL-SOON LEE, University of New Orleans, S. D. MAHANTI, Michigan State University — There is renewed interest in the field of thermoelectrics for power generation. Several promising thermoelectrics are half-Heusler narrow band gap semiconductors. The efficiency of thermoelectric energy conversion depends on the transport coefficients through the figure of merit  $ZT = \sigma S^2 T / \kappa$ . For large  $ZT$ , it is necessary to decrease the total thermal conductivity ( $\kappa = \kappa_l + \kappa_{el}$ ) as well as increase the Seebeck coefficient ( $S$ ) and the electrical conductivity ( $\sigma$ ). To determine  $\kappa_l$  experimentally, one usually subtracts the electronic thermal conductivity ( $\kappa_{el}$ ) from measured  $\kappa$ , using the Wiedemann-Franz law ( $\kappa_{el} = L_0 \sigma T$ ,  $L_0 = 2.45 \times 10^{-8} W\Omega/K^2$ ). To examine the validity of this law in half-Heusler compounds, we have chosen HfCoS as an example. We have calculated the electronic transport coefficients by employing *ab-initio* electronic structure method and the Boltzmann transport equation in HfCoSb. We calculate  $\kappa_{el}$  at constant current  $\mathbf{J}$  ( $\kappa_{el,J}$ ) and constant electric field  $\mathbf{E}$  ( $\kappa_{el,E}$ ) where  $\kappa_{el,J} = \kappa_{el,E} - T\sigma S^2$  which shows a significant deviation from values obtained with Wiedemann-Franz law.  $\kappa_{el,J}$  is much smaller than  $\kappa_{el,E}$  at low carrier concentrations ( $n$ ) and/or at high temperatures ( $T$ ) and the ratio  $\kappa_{el,J}/\kappa_{el,E} \rightarrow 1$  at high  $n$  and/or low  $T$ .

<sup>1</sup>supported by DARPA (HR0011-08-1-0084)

S. D. Mahanti  
Michigan State University

Date submitted: 19 Nov 2009

Electronic form version 1.4