Exploring Thermoelectric Characteristics of Ag-based Chalcopyrites via Deformation Potential Theory: A Non-empirical Range-separated Dielectric-dependent Hybrid Approach

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In the quest for efficient thermoelectric materials, the implementation of a robust design strategy is imperative to optimize electronic and phononic transport properties. In this study, we employ a non-empirical screened dielectricdependent hybrid (DDH) functional in conjunction with semiclassical Boltzmann transport theory to conduct a theoretical investigation of the thermoelectric characteristics exhibited by chalcopyrite compounds [1]. Specifically, our inquiry focuses on the ternary $AgXTe_2$ (X=Ga, In) and quaternary Ag_2ZnSn/GeY_2 (Y=S, Se) systems, emphasizing their potential in harnessing the thermoelectric properties of silver (Ag). Through systematic analysis, we scrutinize the electrical conductivity, Seebeck coefficient, and power factor of these materials. Additionally, we address phonon scattering phenomena [3] using the Elastic constant tensor for electron relaxation time and lattice thermal conductivity. Our investigation establishes the thermoelectric figure of merit, defined by the dimensionless figure ZT = $\sigma S^2 T/\kappa \geq 1$, as a pivotal parameter in characterizing superior thermoelectric materials [2]. To assess the electronic transport characteristics, the deformation potential theory [4]is utilized to analyze the relaxation time. [5, 6]:

$$\tau = \frac{1}{3} \times 2\sqrt{2\pi}\frac{C\hbar^4}{(k_B T m_{\mathrm{dos}^*})^{\frac{3}{2}}}\left(\frac{1}{D}\right)^2 \tag{1}$$

Here, $\hbar$ represents the reduced Planck constant, C denotes the elastic constant, k_B is the Boltzmann constant, $m_{\mathrm{dos}*}$ signifies the effective mass of the density of states (as we focus on a p-type system, we consider only the effective mass of holes), and D refers to the deformation potential energy.

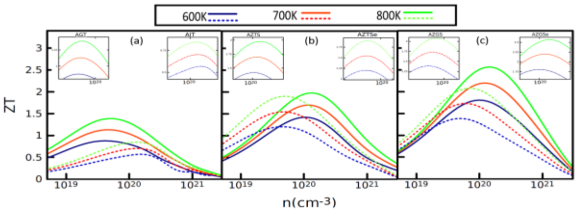

Figure 1: The graphical representation illustrates the computed thermoelectric figure of merit ZT versus carrier concentration across temperatures of 600 K, 700 K, and 800 K for various compounds:(a) Solid lines depict the ZT values for AGT ($AgGaTe_2$), contrasting with the representation of ZT for AIT ($AgInTe_2$) shown by dotted lines. Insets provide individual graphs for AGT and AIT, facilitating the observation of ZT peaks. (b) Solid lines correspond to AZTS (Ag_2ZnSnS_4), while dotted lines represent AZTSe ($Ag_2ZnSnSe_4$). Insets offer segregated graphs for AZTS and AZTSe. (c) The ZT values for AZGS (Ag_2ZnGeS_4) and AZGSe ($Ag_2ZnGeSe_4$)are respectively illustrated by solid and dotted lines. The inset graph provides a comparative analysis of ZT between AZGS and AZGSe.

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