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Thermoelectric Transport Properties of Tin Selenide from First Principles Calculations

The need for new thermoelectric materials that can be used at high temperature for large scale applications has attracted a lot of attention among the researchers over the last few decades. Tin Selenide which is lead-free and relatively cheap has become of interest in the field of thermoelectricity following the reported figure of merit value of 2.6 at 923 K along the b-axis single crystals. In this study we investigated the electronic band structure of SnSe performed using ab-initio calculations done using Quantum Espresso. Thermoelectric properties of the material between the temperature range 300K and 800K were also studied using the BoltzTrap code. Electronic structure calculations were performed using the Generalized Gradient Approximation (GGA) in the form of Perdew-Burke-Enzerhof exchange-correlation functional as implemented in the Quantum Espresso code. An indirect bandgap of 0.625eV was found compared to the experimental value of 0.9eV. Tin Selenide was found to exhibit anisotropic electrical and electron thermal conductivity as well as the Seebeck coefficient. In addition, the material's electrical and electron thermal conductivity was found to be directly proportional to temperature across all the crystal axes. Electrical conductivity was found to be higher on the a & c axes and increased significantly with temperature from 1.233×10^18 at 300K to 4.897×10^18 /Ωms at 800 K on the a-axis and from 1.416×10^18 to 6.49×10^18 /Ωms on the c axis. Electronic thermal conductivity was found to be quite low on the a-axis (8.403×10^12 W/mKs to 1.073×10^14 W/mKs). The Seebeck coefficient was found to be in the range 234 μV/K to 250 μV/K across all axes between 300K to 800K, which is sufficiently high enough for thermoelectric applications. These results show that Tin Selenide exhibits good thermoelectric properties and can perform better at high temperatures for thermoelectric applications.

Primary author: Mr OYOMO, Bill (The Technical University of Kenya)

Co-authors: Ms MUCHIRI, Perpetua (The Technical University of Kenya); Prof. AMOLO, George (The Technical University of Kenya)