Calculation of thermal transport properties for $NbSb_2$ from density functional theory

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Thermoelectric/thermomagnetic materials allow for the transfer of heat by providing current through the material. These materials may be used for refrigeration without any moving parts. However, cooling under 77K using thermoelectric/thermomagnetic effects is not very viable due to the lack of materials with good thermoelectric/thermomagnetic coefficients at that temperature. It has recently been shown that $NbSb_2$ has good thermomagnetic properties at 25K and 5 Tesla. This is seen through the huge Nernst power factor of $3800 \times 10^{-4} W m^{-1} K^{-2}$. Using first-principles calculations it is possible to optimize this value by changing the chemical potential of $NbSb_2$. In this paper, the band structure of $NbSb_2$ will be calculated using density functional theory in the Quantum Espresso software. From these band structures, thermoelectric/thermomagnetic coefficients can be calculated for a range of chemical potentials close to $NbSb_2$'s fermi energy using the nerwann module implemented in wannier90. This has a similar effect to slightly changing the concentration of Nb and Sb as $Nb_{1-x}Sb_{2+x}$. In our work, it has been calculated that the nernst thermopower is around $-60 \mu V K^{-1}$ at a temperature around 25K, magnetic field of 1 Tesla, and chemical potential at the fermi energy. This increases to $-100 \mu V K^{-1}$ at around 22meV above the fermi energy. This study supports Brookhaven National Laboratory's study of quantum materials by providing a possible alternative to cooling materials in a temperature range where quantum effects may be visible. Through the course of this study, I've come to understand semiclassical transport theory and

thermoelectric/thermomagnetic coefficients and how they are defined. I have also understood how to calculate these coefficients from first principles by using wannier90 and nerwann.