NDnano
Notre Dame Nanoscience and Technology

NDnano Summer Undergraduate Research 2022 Project Summary

Student name & home university:

Justin Share – University of Notre Dame

ND faculty name & department:

Professor Gary H. Bernstein – Electrical Engineering
Professor Erik Blair – Electrical & Computer Engineering (Baylor University)

Summer project title: First-principles calculations of thermoelectric properties in monometallic nanothermocouples

Briefly describe new skills you acquired during your summer research:

This summer, I used high performance computing for the first time. Using this skill, I have learned how to write Quantum Espresso files, which I am using to calculate different properties of crystal structures. I have also learned Python's Atomic Simulation Environment (ASE) library to automate the Quantum Espresso calculations.

Briefly share a practical application/end use of your research:

The goal of my research is to learn the thermoelectric properties of different metals and semiconductors at the atomic level. I hope that having a better understanding of these structures' properties will allow researchers to predict what materials can optimize the performance of different devices. The particular device that my research intends to improve upon is the thermocouple in NASA infrared sensors.

50- to 75-word abstract of your project:

NASA infrared sensors are powered by thermocouples which translate a difference in heat into an output voltage. This output voltage is determined by the properties of the metals that make up the thermocouple. This project aims to perform calculations that will provide the thermoelectric properties of different materials. These properties, such as the Seebeck coefficient and thermal conductivity, will discover which materials create the best thermocouples and improve the sensitivity of the infrared sensors.

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One-page project summary that describes problem, project goal and your activities / results:

NASA novel infrared (IR) sensors, called thermoelectrically coupled nanoantennas (TECNAs), are used to detect infrared light. As infrared light hits the nanoantenna, the resonant wavelengths create current flow on the TECNA, which heats the antenna and creates a voltage in a nanothermocouple. The ultimate goal of this project is to improve the sensitivity of these TECNAs by improving the performance of the nanothermocouple.

Thermocouples are made of two metals fused together at a point referred to as the hot junction. As the nanoantenna heats up the hot junction, a voltage is created across the ends of the metallic leads, obeying the Seebeck Effect. The key to the Seebeck Effect is that the leads are two different metals that have unique Seebeck coefficients. The Seebeck Effect is well studied and understood in bulk materials; however, an unexplored phenomenon occurs at the nano level when both thermocouple leads are the same metal.

Prior TECNA experiments showed that it is possible to create the Seebeck Effect between leads if they are the same metal with differing widths. These single-metallic thermocouples function as intended in the TECNAs; however, their performance is difficult to predict because single-metallic thermocouples have never been studied before. The phenomenon that a nanowire's width affects its Seebeck coefficient is unresearched, therefore, there are no theoretical values to compare the TECNA experiments to.

This research intends to resolve this by calculating the Seebeck coefficient and thermoelectric properties of the same metal at different sizes. The ultimate goal is that comparing the thermoelectric properties of different sizes of metal will predict how differing lead widths affect the performance of single-metallic thermocouples.

This project is performing calculations using Quantum Espresso to provide the thermoelectric properties of different materials. These properties include calculating a material's band structure, density of state, thermal conductivity, and optical properties. Knowledge of these properties is crucial because it helps explain the atomic nature of the materials, thereby providing the materials that will maximize the nanothermocouples' voltage output at a specific temperature differential.

Currently, this project is leaving the development stages. Learning the basics of performing Quantum Espresso calculations has taken significant time and practice. However, we have recently begun calculations with different metallic nanowires, and we soon anticipate having Seebeck coefficients to compare to experimental data.