# CALIFORNIA STATE SCIENCE FAIR
# 2013 PROJECT SUMMARY

**Name(s)**

George D. Geng

**Project Number**

**S0611**

**Project Title**

## From Waste Heat to Electricity: Synthesis and Analysis of a New Zintl Phase Compound for Thermoelectric Power Generation

**Abstract**

**Objectives/Goals**

Thermoelectric materials can turn a temperature gradient to electricity. However, to be efficient they need high electrical conductivity and low thermal conductivity. A class of Zintl phases called type-I clathrates have a Si/Ge/Sn framework and extremely low thermal conductivities because of atoms that loosely oscillate in framework voids, disrupting phonons. Their efficiency is low because their electrical conductivity is not too high; however certain d-metals have electrical conductivities orders of magnitude higher than Si, Ge, Sn. The goal of this project is to make a new Zintl phase compound with transition metals incorporated into the framework instead and the same rattling action.

**Methods/Materials**

Formulas of possible phases with a framework containing Cu/Ni and rattling Cs/Rb atoms were predicted from charge-balance requirements (each framework atom must be tetrely-coordinated) in accordance with the Zintl-Klemm bonding concept (relying on the hypothesis that certain transition metals obey the Zintl-Klemm rule). Elements and flux were loaded in the proper ratio into carbonized quartz ampoules, the vessels were vacuum-sealed, and the samples were baked at 850C for 140 hours and then washed to dissolve salts. Powder X-ray diffraction (XRD) data was analyzed. If the analysis indicates a new compound, single crystal XRD data was obtained.

**Results**

Cs(3x)Si(1-x)Cu(x)As(2) and the Rb analog Rb(3x)Si(1-x)Cu(x)As(2) were made in 2 samples; both are new Zintl phase compounds with high electrical conductivity transition metals in the framework. Both contained impurities; however, further syntheses were done until an instance of Cs(3x)Si(1-x)Cu(x)As(2) was created in the pure phase (i.e. alone without other trace compounds). Analysis of the crystal structure and comparison with the traditional clathrate Cs(8)Si(46) revealed a new framework with high concentrations of Cu and As and a similar vibrational structure with Cs atoms in the new compound.

**Conclusions/Discussion**

Cs(3x)Si(1-x)Cu(x)As(2), a new compound with potential for thermoelectric power generation, was synthesized in the pure phase. Additionally, this project demonstrates that the Zintl-Klemm concept holds for certain transition metals, indicating that there may be a class of promising thermoelectric materials with framework-incorporated transition metals and rattling action. Future research will characterize the thermoelectric-figure-of-merit.

**Summary Statement**

This project created a new Zintl phase compound with potential for thermoelectric power generation and demonstrates through the unorthodox application of the Zintl Klemm bonding concept to Cu/Ni that certain transition metals obey the rule.

**Help Received**

Mother helped with the board and printing, used lab equipment at UC Davis under graduate student Juli-Anna Dolyniuk and with guidance of Professor Kirril Kovnir