William Blake, a Romantic, revolted against rationalism famously writing, "To see the world in a grain of sand, And heaven in a wild flower, Hold infinity in the palm of your hand, And eternity in an hour." Blake recognized the unity between the macrocosmic and microcosmic, a oneness I also strive towards as a holistic scientist, creative thinker and universal explorer. This oneness both evokes potential synergies, cooperative interactions creating enhanced effects where the whole is greater than the sum of its parts, which exist in every system and uncovers truths subtler than those of conventional wisdom. Generally, an unconventional perspective employing creativity and follow-through is required to bring these elusive designs into objective reality. Like Blake, Isaac Newton and many others before, I am inspired to think boldly in our own age, always making it a point to have a unique perspective on the big picture with the intent of finding synergies and hidden truths.

Exploration as a means to deepen my understanding of how things work, and work together, has forever been a pillar of my life. I was always going to be an engineer. My parents and grandparents were convinced of this before I knew how to say the word 'engineer'; they decided that I should own my grandfather's NASA jacket adorned with patches carrying the names of NASA and, my last name, Gorham. Upon receiving this gift, my passions focused on Outer Space. As a 3rd grader, I attended Space camp. I remember being in lectures and voraciously soaking in all the information. I participated eagerly, surprising my teachers with my knowledge of the names of astronauts across the Apollo missions. Throughout adolescence and into my present age, my aspirations to explore Outer Space have remained ignited; over the years these aspirations have become flavored with enthusiasm towards astrophysics and energy harvesting as means to deepen my understanding of how the Universe works in hopes of one day being able to explore its expanse first-hand.

My documented research experience and first contributions to entities which will spend time in Outer Space began at NASA Langley Research Center in 2008. Our mechanical systems team's mission was to contribute directly to the development and reliability of the Orion Crew Module, the passenger capsule for a crewed mission to the Moon, an asteroid and Mars. Our primary initiative entailed analyzing the payload's inertial response to the impulsive momentum of inner space flight and the extreme propulsion of take-off. With this analysis, we instructed the positioning of an internal balancing system and iterated between analysis and positioning to develop a least material greatest impact system. Simultaneously, we researched, developed, and fabricated a low-risk method to physically test the moment of inertia of the craft. This technique allowed for ground-based testing as opposed to the typical method of lifting and swinging the craft, an out-dated and precarious approach for such expensive equipment. My team and I presented the culmination of our summer work live on NASA TV to an audience at NASA headquarters in Washington D.C. This experience, my second time participating on a NASA base, was my first of mature, focused, and creative effort on behalf of Space exploration in what I plan to be a lifelong allegiance to NASA with the intention of aiding in the discovery of the subtleties of our Universe.

Seeking personal development to enhance my potential to contribute with an individual perspective to universal exploration, I studied the history of creativity at London's Central St. Martin's College of Art and Design in 2009. Here, I became especially aware of synergetic thinking and the revolutionary power of subtleties. This course in aesthetics proved revelatory for me, a scientist weaned on empiricism and epistemology. Examining juxtaposed dichotomies across disciplines and resolving tensions between the great and minute reaffirmed that science, too, holds truths subtler than those of conventional wisdom. This class was lively and fast moving, focusing on creative methods for generating ideas and offering a selection of approaches to be applied and propagated throughout. Two methods

from this class which continue to facilitate my most productive and creative situations are: the joining of apparent opposites and examining nature thoroughly as a bar for efficient design. Since attending this class I have consciously intertwined these methods and my idea generation process with the motto that repetition is a form of change, and the most prevalent pattern found in nature, a further tenant of the course. Countless areas of my life have became more fulfilling and fruitful since attending this course in creativity, the most tangible are my software coding and modeling abilities. I am able to think with a very open mind about creative solutions to the task at hand while not losing sight of the efficiencies created by structure. The ease with which this aspect of analysis and analytical theory now flows through me has earned coding and modeling a spot in my favorite creative pastimes.

As a holistic scientist, I consistently strive to use creativity to exploit synergies throughout my own academics and research which focuses on energy efficiency as a means to achieve our ultimate goals as conscious beings: quality of life and universal exploration. While my strong macro-engineering education has made me aware of the types of applications and system enhancements demanded for the goal of energy efficiency, my idea generation methods progress my own insight, and stimulate conversation between colleagues, on possible mechanisms to achieve this goal. For example, I have put my holism to use on developing the very unique and independently conceived project, for understanding the subtleties of energy conversion processes of amorphous materials, on which this proposal is based. As a bottom-up, creative, thinker I am inspired by the efficiency of the systems nature creates; having studied nature as a bar for efficient design, I understand that the ultimate efficiencies are created for the system as a whole when synergy is found between all organizational levels, down to the communications between the smallest vibrations. Thus, Patrick Hopkins' Nanoscale Energy Transport Laboratory is the perfect fit for my graduate work and an ideal platform from which to advance energy efficiency for the fulfillment of our goals as conscious beings.

As a young scientist with a full research career ahead, I am convinced that my personal unconventional perspective and embodiment of creativity will determine the content of my contributions. Unveiling the subtleties and interconnectedness of our Universe through direct experimentation, thoughtful theory development, and first-hand exploration will both mold our future as a species and affect our relationship with the Cosmos. I am thrilled to be an engineer during this age of compounding newfound physical understanding; I am prepared to collaborate and contribute my personal perspective. We will go far during this age – to Mars and beyond.

Project Narrative - NSTRFP - Optimizing Materials for Energy Harvesting on Interplanetary Return Missions - Caroline S. Gorham - 8 November 2013

1 Project Statement

Manned interplanetary missions will only be desirable once the ability to return is established. Even using improved fuel technologies we have not resourced the fuel requirement for return missions to our nearest terrestrial neighbors. Energy harvesting in Outer Space or on another planet is imperative for return mission success, as it is impossible with current Earth-based fuel technologies to supply an outgoing mission, to even our closest neighbor planets, with enough fuel for return. Thermophotovoltaic (TPV) devices, with a theorized maximal efficiency of 85% conversion of incident sunlight to electricity [1, 2], are ideal for such harvesting. **Thus, the work I propose will investigate performance parameters of select TPV materials. Specifically, I will study how the optical absorption, thermal emission, energy conversion efficiencies, and thermal transport properties are related to the structural features of TPV materials in the presence of photon wavelengths abundant in the Universe.** Through an in-depth, computational and theoretical study of the relationship between amorphous material structure (i.e., atomic density and kinetics of the population of localized states [3]) and the optical absorption, thermal emission, electronic conversion and thermal transport properties will be determined. The results will establish the governing materials physics to further guide material selection and device design for efficient electromagnetic harvesting cells to be used for constant refuel on interplanetary missions.

2 Introduction and Overview of Proposed Work

Solar energy is a clean and renewable energy source consistently available in Outer Space, on Earth and on neighboring terrestrial planets. Optimization of electromagnetic harvesting devices that convert light into electricity offers the potential for a perpetual and reliable source of fuel both on Earth and on interplanetary missions. It is theorized that TPV devices, which ideally absorb and convert all incident solar radiation to a spectra of thermal emission finely tuned for conversion to electricity by another photovoltaic (PV) cell, can reach a maximum efficiency of 85% [1, 2]. The effects of component material morphology (i.e., amorphous or crystalline) [4, 5, 6, 7], material family (i.e., inorganic, organic, or hybrid) [8, 9, 10, 11], and processing [12, 13] on performance parameters affecting ultimate power conversion of these devices continue to be investigated. Yet, we remain far from the theorized maximum efficiency of these devices, thus, further investigation of the structural parameters of TPV materials is warranted.

The intention of this proposed project is to determine the physics behind the optimization of energy conversion via molecular structure to aid in the development of energy harvesting materials that are functionally optimized for yield and efficiency in Outer Space and on Mars. Through coupled theoretical and computational thrusts, this initiative will elucidate relationships between energy absorption and transport and the microstructural details of amorphous systems, i.e., atomic density and kinetics of the density of localized states. The thermal transport and electronic scattering properties of computationally-constructed structures will be simulated with both classical methods via molecular dynamics, and through quantum mechanical derivation with lattice dynamics, the Boltzmann transport equation, and a non-equilibrium Green's function formalism. Development of models detailing the dependences between the structural aspects of the amorphous systems and both energy absorption and thermal transport energy will support these studies.

This modeling initiative, with joint computational and theoretical components, will address the following questions focusing on the independent and dependent optimization parameters outlined in Fig. 1, with the aim of developing theory to improve energy harvesting capabilities:

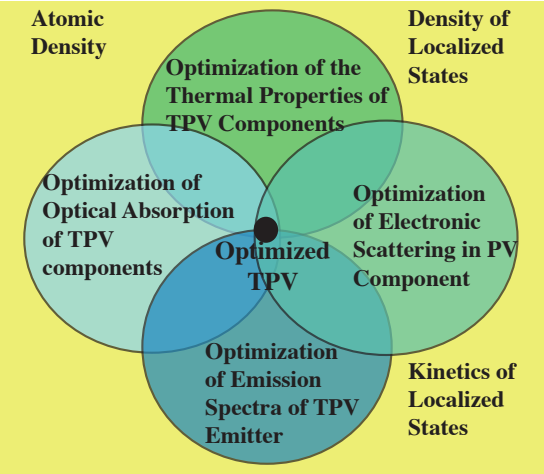

FIGURE 1. Schematic pictorially representing the independent parameters that will be investigated to determine the structural arrangements that simultaneously optimize optical absorption, electronic conversion, and the emission spectra of TPV materials.

1. **Atomic Density:** What are the characteristic atomic-level length scales of amorphous materials that give rise to peak electromagnetic energy absorption (of the full spectrum or of finely tuned spectra) and electronic conversion? Can finely tuned porosity or local differences in atomic density, provide pathways for electron transfer while maintaining efficacy of optical absorption? To what degree can the thermal emission spectra and the thermal transport properties be optimized by changes to material structure at multiple length scales?

2. **Density and Kinetics of Localized States:** What can be understood about the kinetics of localized states from understanding of the atomic-level length scales of order and disorder in amorphous materials? What magnitude of change to performance parameters can be realized through tuning these structural details? What causes the alteration, i.e., how do the density of localized vibrational states affect the scattering of electrons and their ease of separation from the valence band into the conduction band? Do functionalization or polymerization affect these relationship? Can the vibrations in organic semiconducting materials be distinguished as due to long-range order, medium-range order and short-range order, what distinguishes them? Do high-momentum vibrations in organic semiconducting polymers exist on a fractal network in wave-space? What is the relationship between the fractal dimension of the network high-momentum vibrations in real-space, as the ensemble of vibrations on the fractal network, population of localized vibrational states, and energy harvesting performance?

To provide a mission-specific description, the materials chosen for this investigation are not only widely-known to be scientifically interesting materials, due to their unique electronic and vibrational systems [], but also have proven facility for use on interplanetary missions [14]. We will investigate organic semiconducting polymers including but not limited to: PCBM, P3HT, and P3HT:PCBM blend thin films. Due to their small band gaps [15] these materials have an extremely high capacity for absorption in the visible and near-IR spectra [16], wavelengths abundant on the Martian surface and in interplanetary space [17]. They also offer low thermal conductivities [18] and controllable fractal-dendtritic growth [19, 20, 21]. With further improvements to energy conversion efficiency, these amorphous organic materials offer cost-effective and reliable alternatives to current state-of-the-art TPV device materials.

3 Background

3.1 Radiation on Mars and in Outer Space

Beyond Earth's protective atmosphere there exists an abundance of radiation. Radiation, defined as energy in transit, may be classified as either non-ionizing or ionizing dependent on its magnitude of energy. More specifically, ionizing radiation carries enough energy to eject electrons from matter that

it interacts with. While it is conceivable that all forms of radiation may be harnessed for usable energy in the form of heat, electricity, or pressure, the energy harvesting device to be improved upon by this proposed research readily converts only non-ionizing radiation. Furthermore, the functionality of TPV devices may be negatively affected by ionizing radiation and, therefore, it is expected that the device will be properly shielded from such incident rays and particles; the necessary shielding is not an initiative of this proposal.

The intensity and spectra of non-ionizing radiation present on the Martian surface differs from that in orbit or, as a point of reference, on the Earth's surface. In orbit or in interplanetary space, the blackbody radiation of the Sun pervades across most of the electromagnetic spectrum (gamma rays are converted to lower energy photons before reaching the Martian surface) with the limiting factor on intensity of the spectra being inversely proportional to the distance from the source. At Mars, the absorbance and collisions that the Sun's irradiance will have experienced on its travel leaves the density of incident solar radiation to be approximately half that reaching Earth's surface. Based on recent observations from the Curiosity rover on Mars, the overall radiation dose rate is also approximately half that of the average experienced on the cruise to the planet; this is explained by the rover being on the planet versus in space where it would have exposure to radiation from all directions. However, despite the diminished radiation rate experienced on Mars, the planet's minimal atmosphere, consisting mainly of CO_2 and dust, does not abundantly scatter and absorb solar radiation in the visible spectra [17]. Additionally, the planet's lack of an ozone (O_3) layer allows for drastically lower UV absorption and scattering than compared to that of Earth's atmosphere. It has been reported that the surface of Mars, during periods of daylight, receives a total UV flux between 200-400 nm that is comparable to that incident upon the Earth's surface [22]. However, CO_2 clouds do readily reflect and absorb wavelengths less than 204 nm [17, 22, 23] and a small fraction of wavelengths in the IR range [24]. Likewise, these clouds partially reflect the upwelling of IR radiation from the planet surface back towards the surface [25]. Focusing on the wavelengths prevalent on the Martian surface, this study will investigate a range of frequencies in the near-UV, visible, and near-IR spectra.

3.2 Thermophotovoltaic Technology

TPV devices consist of an absorber to collect and convert non-ionizing radiation to thermal emission and a PV cell that converts the received wavelengths into electronic energy. Ideally, the absorber will absorb all wavelengths and convert them, without loss through waste heat and emission, to a wavelength spectra finely tuned for absorption by a PV cell. Ideally, this wavelength spectra will be completely absorbed by the PV cell that is optimized to convert this incident radiation to electronic energy. This electronic conversion is optimal when the excited electrons remain in the conduction band for long enough to extract usable current while minimizing electron scattering, caused by waste heat, and heating effects. For ideal components with no optical losses and only radiative recombination in the solar cell, theoretical maximal efficiencies are found to be 85% for full concentration of the incident sunlight on a black absorber [1, 2]. Therefore, the initiative of this proposal is to achieve near blackbody optical absorption, finely tuned thermal emission, long electron excitations, minimal electron scattering, and efficient waste heat removal through exploiting the structural morphology of amorphous TPV materials.

3.3 Organic Polymer Semiconductor Thin Films

Organic polymer semiconducting materials exhibit many electronic properties and manufacturing advantages that make them ideal for use as energy conversion materials. Additionally, thin film morphology offers improved flexibility [26, 27], manufacturing cost reduction [26, 27], and control over the fractal dimension of the material [19]. These materials have small band-gaps, absorbing and emitting in the visible and very near-IR spectra, making them ideal candidates for energy harvesting on Mars and in

Outer Space. Much work has been done to optimize the parameters affecting overall power conversion efficiencies, these being: photon absorption [4, 6, 28, 26], electron excitation [10, 11, 26, 7, 29, 30, 28], diffusion of the electron-hole pairs to their respective electrodes for collection [11, 29, 30, 28, 26], thermal emission spectra of the emitter [31, 32, 33] and waste heat removal [34]. However, these parameters are not yet fully optimized. The current low TPV power conversion efficiencies of organic semiconductor materials can be attributed mainly to incurred resistances due to improperly spaced electron energy levels for the charge generation, transportation, and collection at the TPV electrodes caused by poor spatial geometries [35, 36].

4 Technical Approach and Methods

4.1 Overview of Approach and Methods

By conducting both classical and quantum mechanical simulations, and by modeling energy conduction properties, this initiative aims to isolate the effects of atomic structure and microstructure on the energy conversion performance of organic semiconducting polymers. Specifically, the interplay between atomic density, the density of localized vibrational and electronic states, and: vibrational-electron scattering, transition between localized and delocalized electronic states, and photon absorption/emission will be investigated. Computational tools will be selected based on the accessible length scales and transport physics. Models generated alongside computation will incorporate results with the aim of isolating the role of microstructure on the properties of interest. It is anticipated that theoretical breakthroughs pertaining to energy conversion in organic semiconducting polymers will stem from the pairing of computation, atomistic and quantum mechanical, and theoretical modeling.

Briefly, molecular dynamics simulations, obeying classical Newtonion mechanics and providing atomic-level trajectories, and lattice dynamics, whereupon the vibrational modes are quantized, will facilitate the calculation of both the scattering times of the vibrational states and the relative densities of non-localized and localized vibrational states in the organic semiconducting polymer systems. Modeling of the thermal and electronic conduction properties of the material, which includes the theoretical scattering times and density of states functions as parameters, will be conducted simultaneously. Electron-phonon coupling, and subsequent relaxation of the electron, at the temperatures pertaining to interplanetary travel and the Martian surface will be isolated and interrogated with the assistance of the data from classical simulations, the theoretical models and quantum mechanical non-equilibrium Green's functions. Non-equilibrium Green's functions computations driven by first principles density functional theory calculations are fundamental in that they construct the material from the electronic level using quantum mechanics. This technique will be employed to determine the channels of least resistance felt by the electrons within the system. By exploring the science pertaining to the energy modes on the photovoltaic surface, in conjunction with calculations of the vibrational modes of the system, photon absorption and emission will be calculated. Again the effort will be twofold: to describe the science behind the energy transport and microstructure of the material, and to generate theoretical models that describe the phenomena.

4.2 Atomistic and Quantum Mechanical Methods/Simulation

Prior to predicting material properties, the samples of interest must be prepared in the computational environment. Atomic position information for fullerenes are available. The molecular structure will be constructed in Avogadro, a molecular structure editor. Subsequently, the simulation cell to be investigated for the purposes of this study will be generated. Initial investigations of the isolated molecules will generate baseline material property information from which the effects of complexities of material and electronic structure can be calibrated.

The vibrational thermal conductivity, scattering times, and density of states will be produced using both molecular dynamics and lattice dynamics. Thermal conductivity will be predicted using the Green-Kubo method in molecular dynamics simulations. Scattering rates obtained by molecular dynamics will be compared to those obtained using lattice dynamics calculations and structure factor techniques. The lattice dynamics calculations will also be performed using input from density functional theory calculations, leading to a refined predictions of the vibrational density of states and the inclusion of quantum effects at low temperatures. However, it is a more time-consuming technique than mfaolecular dynamics and the use of computational resources must be paired with necessity. That said, scattering function calculations will be completed within the first principles framework and compared with the classical results from molecular dynamics.

Quantum mechanical non-equilibrium Green's functions will be used to study the effects of specific structural arrangements on electron scattering. The trends determined with the non-equilibrium Green's functions approach will be directly compared to the trends observed in theory and modeling to determine the intricacies in the interplay between atomic arrangement and electron excitation and recombination on an atomistic level.

4.3 Model Development

In parallel and in complement to the computation, a second thrust of this initiative will be theoretical model development. Two benefits that theoretical models provide are: the calculations are quick and the parameters or contributions of interest can be easily isolated over temperature regimes. The primary focus of the model development will be on the thermal transport and electronic scattering properties of organic semiconducting materials. Initially, this thrust will aim to isolate the vibrational scattering terms and vibrational densities through modeling of the thermal conductivity and heat capacity by describing the vibrational system of electrically insulating materials. This general model will then be extended to predict the thermal properties, thermal conductivity and heat capacity, of organic semiconducting materials. In doing so, not only will the electronic conductivity be calculated through application of the Wiedemann-Franz law, electronic and vibrational mode scattering rates, and mode populations at the temperatures of interest will be found. Because of the atomic-level construction of these models, this information will allow for general prediction of the effect of macromaterial properties on both the thermal and electrical conduction in organic semiconducting material systems. To incorporate the computational developments into this modeling thrust, progress will be made to introduce the effects of functionalization and blend-mixing into the theoretical models.

5 Work Plan

Following the work plan shown in Fig. 2, Ms. Gorham will present results at acclaimed physical sciences and engineering symposia and conferences. Ms. Gorham's research will result in numerous high impact publications in advanced materials, chemistry, physics and engineering journals. The project management plan includes several interactions with supervisors and colleagues at different frequencies and formalities. Ms. Gorham will meet weekly with her Ph.D. supervisor, Dr. Alan McGaughey, will stimulate communication with NASA contacts through informal debriefs and a presentation of annual reports. Furthermore, Ms. Gorham plans to spend time on-site at appropriate NASA facilities to work alongside lead researchers to advance the project throughout the various states of this initiative.

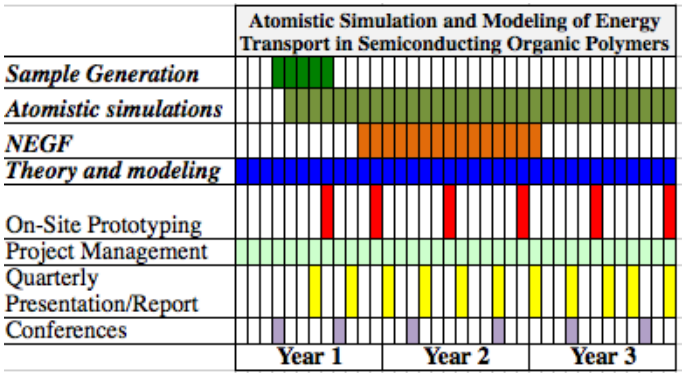

FIGURE 2. Project timeline.

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Degree Program Schedule – Caroline S. Gorham

Enter Program – Summer 2012

Summer Semester 2012
- Independent Study, Physical Chemistry I and II (3 semester credits)

Fall Semester 2012
- Engineering Analysis I, Partial Differential Eqns. (3 semester credits)
- Thermomechanics (3 semester credits)

Spring Semester 2013
- Electronic, Magnetic and Optical Properties of Materials (3 semester credits)
- Engineering Analysis II, Partial Differential Eqns. (3 semester credits)
- Computation as a Research Tool (3 semester credits)

Fall Semester 2013
- Physics of Materials (3 semester credits)
- Electronic and Crystal Structure of Materials (3 semester credits)

Spring Semester 2014
- Density Functional Theory (3 semester credits)
- Classical Simulation of Materials (3 semester credits)

Fall Semester 2014
- Numerical Methods (3 semester credits)
- Quantum Mechanics (3 semester credits)

Qualifying Exams – Spring 2015

Spring Semester 2015
- Thermal Transport in Nanomaterials (3 semester credits)

Doctoral Proposal – Fall 2015

Fall Semester
- Statistical Mechanics (3 semester credits)

Doctoral Defense – Fall 2016

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Education

Carnegie Mellon University, Dept. of Mechanical Engineering — **Pittsburgh, PA**
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Thesis Work: "Thermal properties of semiconducting amorphous materials" — – 201X

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Thesis Work: "Optimal polymerization of silica nanoparticles minimizing size and size dispersion"

Central St. Martin's College of Art and Design — **London, UK**
Developing Your Creativity — Winter 2009

Stanford Graduate School of Business — **Palo Alto, CA**
Summer Institute for General Management — Summer 2009

Funding

NASA Space Technology Research Fellowship — 2013 – 201X
Proposal Work: "Optimizing materials for energy harvesting on interplanetary return missions"

Papers

2. B. M. Foley, C. S. Gorham, J. C. Duda, R. Cheaito, C. J. Szwejkowski, C. Constantin, B. Kaehr, and P. E. Hopkins, "Thermal conductivity of water insoluble protein films: anharmonic interations of vibrations in a fractal structure," – to be published in *Journal of Physical Chemistry Letters*.
1. A. Godeke, P. Bish, D. R. Dietderich, C. S. Gorham, A. R. Hafalia, H. C. Higley, N. L. Liggins, M. G. T. Mentink, and G. L. Sabbi, "Novel methods for the measurement of critical current of superconducting wires," – *AIP Conference Proceedings*, vol. **1435**, no. 1, pp. 209-216, 2012.

Poster Presentations

2. C.S. Gorham, B.M. Foley, J.C. Duda, R. Cheaito, C.J. Szwejkowski, C. Constantin, B. Kaehr, and P.E. Hopkins, "Thermal conductivity of water insoluble protein films: anharmonic coupling in a fractal structure," – *ASME-IMECE,* 19 November 2013, San Diego, CA.
1. C.S. Gorham, K. Hattar, R. Cheaito, T. Beechem, J.C. Duda, J.F. Ihlefeld, D.L. Medlin, E. S. Piekos and P.E. Hopkins, "Effects of surface treatments on thermal boundary conductance across Al/Si interfaces," – *MRS Spring Exhibit,* 3 April 2013, San Francisco, CA.

Experience

Raytheon Company (IIS): System Engineer and Integrator — **Aurora, CO** 2010 – 2011
LBNL: DOE Science Internship: Superconducting Magnet Group — **Berkeley, CA** Summer 2010
NASA Langley: Mechanical Systems Engineering Intern: Mass Properties — **Hampton, VA** Summer 2008

Additional Interests

- Advanced level MATLAB modeling
- Member of NSPE, SWE, ASME, MRS, IMechE and IEEE associations
- Mechanical EIT

References can be made available upon request.