**roject Title:** Predicting Thermal Transport in Nanostructured Materials using *Ab-Initio* Calculations

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*The objective of my research is to build a robust, accurate, and efficient computational framework for predicting the thermal transport properties of nanostructured materials using phonon properties calculated from first principles quantum mechanical calculations.*

Controlling thermal transport is crucial for optimizing the performance, reliability, and lifetime of devices for electronic, optoelectonic, and energy conversion devices. For example, the ideal material for thermoelectric energy conversion has a low thermal conductivity, while high thermal conductivity is needed to remove the excess heat generated in light-emitting diodes (LEDs) [1,2,3]. Both of these emerging technologies offer the promise of reducing energy consumption at a national scale, but suffer from low efficiencies related to thermal transport. Nanostructures (e.g., thin films, nanowires, superlattices) offer an intriguing opportunity to the tune thermal transport properties of the component materials, allowing for new design strategies for tailored device operation.

Thermal transport in a semiconductor is controlled by phonons, quanta of energy associated with atomic vibrations. Transport in a nanostructured material can be described by an effective thermal conductivity, which can be very different than the bulk values available in common references. The effective thermal conductivity of a nanostructure is lower than the bulk value due to the scattering of phonons with the system boundaries. It is these boundary effects that provide the opportunity for controlling thermal conductivity by engineering the device nanostructure [3].

Developing design strategies for controlling thermal conductivity through nanostructuring requires atomic-level analysis. The required inputs are the nanostructure geometry, phonon properties, and a boundary scattering model. The nanostructure geometry is my design objective. Boundary effects can be accounted for using tools developed by my research group, the Nanoscale Transport Phenomena Laboratory [4,5]. The critical inputs are the phonon properties (specific heat, velocity, and lifetime). These can be predicted using molecular dynamics simulations and lattice dynamics calculations. While the classical approaches typically used are conceptually simple and computationally inexpensive, they are poor at reproducing experimental measurements. To obtain more accurate phonon properties, I propose to use *ab-initio* (from first principles) calculations, which include quantum mechanical effects [6]. I am developing a new algorithm to calculate phonon properties, which, while slightly more computationally demanding than existing algorithms, is conceptually much simpler and will be accessible to a wide range of engineers and scientists [6]. I will then use the *ab-initio* phonon properties obtained from my new algorithm to engineer nanostructures with tailored thermal conductivities, with a focus on reduced thermal conductivity silicon-germanium materials for thermoelectric energy conversion devices.

***Obj. 1****: develop and validate algorithm for predicting phonon properties from Ab-Initio calculations.*

***Obj. 2****: use ab-initio phonon properties to engineer thermal transport in nanostructures.*

***Obj. 3****: publish results to inform experimentalists and engineers of design strategies.*

[1] D.G. Cahill et al., *J. Appl. Phys.* **93**, 793 (2003). [2] E. Pop et al.**,** *J. Electron. Packag*. **128**, 102 **(**2006**)**.

[3] A.I. Hochbaum et al.,*Nature* **451**, 163-167 (2008). [4] J.M. Larkin et al., *Phys. Rev. B* (submitted).

[5] J. E. Turney et al., *Phys. Rev. B* **79** 064301 (2009). [6] K. Esfarjani et al., , *Phys. Rev. B* 77, 144112 (2008).