

Project Title: Controlling Thermal Transport in Nanostructured Materials using *Ab-Initio* Calculations

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Project Description: *The objective of this project is to build a robust, accurate, and efficient computational framework for predicting thermal transport in nanostructured materials using Ab-Initio phonon properties.*

Controlling thermal transport is crucial to the performance of nanostructured devices. The efficiency of high energy consumption devices such as semiconductor thin films, solidstate memory, and semiconductor light-emitting diodes depends on optimizing thermal transport [1,2]. Thermal transport in nanostructures is controlled by an effective thermal conductivity, which can be very different than bulk. The effective thermal conductivity of thin films is reduced over the bulk, which limits their ability to effectively remove waste heat [2]. For thermoelectric energy generation - the transformation of waste heat into useful electricity - the ideal thermoelectric material thrives from reduced thermal conductivity [3]. The thermal conductivity of nanostructures is altered by boundary effects as dimensions are reduced. These boundary effects provide the opportunity to control thermal conductivity by engineering the device nanostructure [3].

Controlling thermal conductivity through nanostructuring requires atomic level analysis using molecular and lattice dynamics simulations. Boundary effects can be accounted for using the tools developed by our group, the Nanoscale Transport Phenomena Laboratory (NTPL) [4,5]. Bulk phonon properties are used as the input for the boundary analysis. Phonons are quantized atomic vibrations that exists in a crystalline material. The phonon properties are predicted using molecular and lattice dynamics simulations, which model a system at the atomic level. Classical atomistic simulations are conceptually simple and computationally inexpensive, but are poor at predicting phonon properties. To make accurate predictions, we use *Ab-Initio* (from first principles) calculations, which include the effects of quantum mechanics [6]. A simplified algorithm is used to calculate the phonon properties, which is computationally more demanding than other algorithms but is conceptually much simpler [6]. The *Ab-Initio* phonon properties will then be used to engineer nanostructures with tailored thermal conductivities for applications in semiconductor and thermoelectric devices.

Research Plan

Objective 1 (months 1-3): *develop and validate algorithm for predicting phonon properties from Ab-Initio calculations.*

Objective 2 (months 3-6): *apply Ab-Initio phonon properties to boundary scattering analysis to engineer thermal transport in nanostructures.*

Objective 3 (months 6-): *publish results to inform experimentalists and engineers of design strategies.*

[1] D.G. Cahill et al., "Nanoscale thermal transport", *J. Appl. Phys.* **93**, 793 (2003).

[2] E. Pop et al., "Thermal Phenomena in Nanoscale Transistors", *J. Electron. Packag.* **128**, 102 (2006).

[3] A.I. Hochbaum et al., "Enhanced thermoelectric performance of rough silicon nanowires", *Nature* **451**, 163-167 (2008).

[4] J.M. Larkin et al., "Comparison and Evaluation of Spectral Energy Methods for Predicting Phonon Properties", *Phys. Rev. B* (in submission).

[5] J. E. Turney et al., "Predicting Phonon Properties and Thermal Conductivity from Anharmonic Lattice Dynamics Calculations and Molecular Dynamics Simulations", *Phys. Rev. B* **79** 064301 (2009).

[6] K. Esfarjani et al., "Method to extract anharmonic force constants from first principles calculations", *Phys. Rev. B* **77**, 144112 (2008).