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# Rational Nanostructure Design for Efficient Energy Devices

**Abstract:** Experimental and computational works suggest that the phonon-phonon scattering in silicon nanostructures with dimensions greater than 50 nm is bulk-like. Inspired by this finding, I will describe a Monte Carlo technique for predicting the thermal conductivity of an arbitrary nanostructure. The only required inputs are the bulk phonon properties, the system geometry, and a boundary scattering model. Using phonon properties obtained from density-functional theory calculations, I will demonstrate and validate the technique through application to nanoporous silicon thin films. By comparing to existing experimental measurements, the postulated existence of coherent phonon effects will be assessed.

## Alan McGaughey

**Associate Professor**

**Dept. Mechanical Engineering**

**Carnegie Mellon University**

**Pittsburgh, PA 15213**

**Biography:** Alan McGaughey is an Associate Professor in the Department of Mechanical Engineering at Carnegie Mellon University and a Harrington Faculty Fellow at UT Austin for 2012-13. He was the Struminger Junior Faculty Fellow in 2009 and won a Air Force Office of Scientific Research Young Investigator Program award in 2009. He holds B. Eng, M. A. Sc., and Ph. D. degrees in mechanical engineering from McMaster University, the University of Toronto, and the University of Michigan. Before starting at Carnegie Mellon in 2005, he spent a year as a post-doctoral fellow in the Materials Science and Engineering Department at the University of Florida. His research group, the Nanoscale Transport Phenomena Laboratory, is supported by the NSF, AFOSR, and DARPA.