Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Theoretical study of lattice thermal conductivity in Si clathrate materials JIANJUN DONG, XIAOLI TANG, Physics Department, Auburn University — Recent experiments have shown that Si and Ge clathrate crystals are promising candidates as high ZT thermoelectric materials because of their glass-like low thermal conductivity. Based on a detailed *ab initio* calculation of equilibrium statistical properties, we conclude that the distinct structural differences in the diamond-structured Si (d-Si) and the type-II Si clathrate (Si_{136}) only lead to some minor differences in the equilibrium thermal properties in the two tetrahedrally bonded Si phases. In this talk, we will present our recent calculations of non-equilibrium thermal transport properties of d-Si and Si_{136} crystals, based on the statistical linear response theory. The key step of our calculation of lattice thermal conductivity (κ) is to evaluate the fluctuation-correlation relation of bulk heat currents at equilibrium conditions. In the current study, we have adopted the molecular dynamics (MD) simulation techniques, using large atomic supercell models and the Tersoff potential. Our results suggest that the cage-like open framework of clathrate crystals will lead to a factor of 5-8 reduction in thermal conductivity. The MD simulation results are also discussed in the context of the simple kinetic transport model. The "anomalous" oscillation feature in the correlation functions of clathrate materials is explained.

Jianjun Dong
Physics Department, Auburn University

Date submitted: 20 Nov 2006 Electronic form version 1.4