Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

First Principles Studies of Thermoelectric Figure of Merit of Si and SiGe Nanowires[1] TRINH VO, JOHN REED, ANDREW WILLIAMSON, Lawrence Livermore National Laboratory, YING MENG, TIM MUELLER, MARIA CHAN, GERBRAND CEDER, Massachusetts Institute of Technology , GALLI GIULIA, University of California at Davis, LAWRENCE LIVERMORE NATIONAL LABORATORY TEAM, MASSACHUSETTS INSTITUTE OF TECHNOLOGY COLLABORATION, UNIVERSITY OF CALIFORNIA AT DAVIS COLLABORATION — We present predictions of the thermoelectric figure of merit (ZT) of Si_xGe_{1-x} nanowires based on Density Functional Theory calculations and cluster expansion optimizations. The electrical conductivity, σ, and Seebeck coefficient, S, were obtained using the Boltzmann transport equation in the relaxation time approximation, and first principles, electronic structure calculations. The thermal conductivity was computed using classical molecular dynamics runs. A range of SiGe nanowires with different Ge concentrations and Ge distributions were investigated. We found that the transport coefficients σ, S, and thus ZT strongly depend on the wire growth direction, surface structure, and Ge concentration, and Ge distribution. These parameters were varied to obtain a nanostructure with an optimal, high figure of merit above 2 or 3, depending on the electronic doping.

[1]This work was performed under the auspices of the U.S. Dept. of Energy at the University of California/Lawrence Livermore National Laboratory under contract no. W-7405-Eng-48.

Trinh Vo
Lawrence Livermore national Laboratory

Date submitted: 20 Nov 2006 Electronic form version 1.4