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First Principles Studies of Phonon Dispersion and Lattice Thermal Conductivity of Silicon Nanowires TRINH VO, TADASHI OGITSU, ERIC SCHWEGLER, LLNL, GIULIA GALLI, UC Davis — We present phonon dispersions of Si nanowires using *ab initio* and linear response theory. The effects of nanowire surface structures, growth directions, and quantum confinement on phonon dispersions and phonon confinement are also discussed. The thermal conductivity of Si nanowires using the obtained full dispersion curves are also evaluated, using Boltzmann Transport Equation. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory in part under Contract W-7405-Eng-48 and in part under Contract DE-AC52-07NA27344.

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