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Comparisons of electronic transport properties computed via classical and quantum molecular dynamics HEATHER WHITLEY, CHRISTIAN SCULLARD, LORIN BENEDICT, Lawrence Livermore National Laboratory, MICHAEL DESJARLAIS, Sandia National Laboratory, FRANK GRAZIANI, Lawrence Livermore National Laboratory, CIMARRON COLLABORATION — We have applied the ddcMD molecular dynamics (MD) code to the computation of the electrical conductivity and thermal conductivity of hydrogen plasmas at several points in phase space. Quantum mechanical effects on the electronic degrees of freedom are incorporated through the use of temperature-dependent statistical potentials. In order to examine the validity of this approach, we make comparisons with results from quantum MD simulations. We find that, while the electrical conductivities computed via classical MD are in reasonably good agreement with the quantum MD calculations, the thermal conductivity computed via classical MD is lower than the quantum MD result by a factor of 2-3. The Lorenz number determined from the classical MD is a factor of 2-3 lower than the Spitzer prediction. Similar discrepancies with Spitzer were also observed by Bernu and Hansen. LLNL-ABS-640881 This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344. Lawrence Livermore National Security, LLC.

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