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The Thermal Conductivity of National Ignition Facility Target Materials D.E. HANSON, L.A. COLLINS, J.D. KRESS, Los Alamos Nat. Lab, M.P. DESJARLAIS, Sandia Nat. Lab. — Using quantum (finite-temperature density functional theory) molecular dynamics (QMD), we performed simulations of several important materials in the Inertial Confinement Fusion-National Ignition Facility nominal target designs, comprising various mixtures of proposed ablator materials (Be or CH) with the DT fuel. Simulations were done over a range of temperatures between 5 eV and 20 eV, at densities between 7.5 and 14 g/cc. The QMD program (VASP) produces the Kohn-Sham orbital wavefunctions and associated eigenenergies from which we determine both the electrical and thermal conduction properties from a Chester-Tellung-Kubo-Greenwood formulation. We find that the thermal conductivity is not sensitive to modest density variations but is quite sensitive to the mix fraction. We find that the thermal conductivity of mixed systems can be approximated to within 20% by the Faber-Ziman equation. We also compare our QMD results to the Hubbard and Lee-More thermal conductivity models. For the conditions of our simulations, the Hubbard model is in reasonable agreement with the QMD results.

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