Abstract Submitted
for the DFD14 Meeting of
The American Physical Society

Thermal conductivity and heat capacity of n-decane and n-hexadecane through molecular simulations JOHN SHELTON, Carnegie Mellon University — Atomistic molecular dynamics simulations were carried out at equilibrium to calculate the constant pressure heat capacity and thermal conductivity of n-decane and n-hexadecane within the range of ambient to extreme temperature and pressure conditions (i.e. up to 500 °F and 35,000 psi). Both a computationally efficient united-atom force field and an all-atom force field were employed in this investigation. A quantitative comparison of the results was performed against experimental values and values predicted from a high temperature - high pressure perturbed chain - statistically associated fluid theory (HPHT PC-SAFT) model. Analysis of the intra- and inter-molecular structure of the fluid as well as its dynamical characteristics were performed.

John Shelton
Carnegie Mellon University

Date submitted: 01 Aug 2014 Electronic form version 1.4