

Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Structural investigation and shock Hugoniot calculations of methane under high temperatures and pressures BENJAMIN SHERMAN, California State University, Northridge, BURKHARD MILITZER, HUGH WILSON, University of California, Berkeley, DAYANTHIE WEERARATNE, California State University, Northridge — The behavior of methane under pressures and temperatures spanning 0.02-7.75 Mbar and 300-30,000 K was studied using density functional molecular dynamics. The structural properties of fluid and crystalline methane were analyzed with simulations at various (P,T) conditions. These simulations were also used to calculate the shock Hugoniot curves of methane for a range of initial densities between 0.4-0.57 g/cc. These curves allow us to make predictions of state and phase that correspond to future methane shock experiments.

Benjamin Sherman
California State University, Northridge

Date submitted: 27 Nov 2010

Electronic form version 1.4