Abstract Submitted for the MAR14 Meeting of The American Physical Society

Physical Properties of Supercritical Silica CARL GREEFF, DANIEL SHEPPARD, Los Alamos National Laboratory — Supercritical states of silica – states lying above the vapor dome – are produced on release from strong shocks applied to solid quartz, as may have occurred in a planetary impact that formed the moon. These states are also reached in shocks applied to highly porous aerogels. In the supercritical region, ion-ion correlations and thermal excitation of electrons are significant and non-trivial. Models used in wide-ranging equations of state such as Sesame generally have simplified physics in this region. We present results from extensive quantum molecular dynamics simulations for the equation of state and optical properties of supercritical silica. The simulations are found to reproduce the aerogel Hugoniot very well. We examine the nature of the ion correlations and electronic spectrum with an eye toward improving equation of state models in this difficult region.

Carl Greeff Los Alamos National Laboratory

Date submitted: 13 Nov 2013

Electronic form version 1.4