Abstract Submitted
for the SHOCK19 Meeting of
The American Physical Society

Critical point, liquid-vapor coexistence, and melting of Mg_2SiO_4 from ab-initio simulations[1] JOSHUA TOWNSEND, High Energy Density Physics Theory, Sandia National Laboratories, Albuquerque, NM 87185, GIL SHOHET, Department of Aeronautics Astronautics, Stanford University, Stanford, CA 94305, LUKE SHULENBURGER, High Energy Density Physics Theory, Sandia National Laboratories, Albuquerque, NM 87185, MICHAEL DESJARLAIS, Pulsed Power Sciences, Sandia National Laboratories, Albuquerque, NM 87185 — We report density functional theory-based molecular dynamics calculations (DFT-MD) of Mg_2SiO_4 liquid and vapor across the liquid-vapor coexistence boundary that spanned 0.22-3.22 g/cc in density and 5000-10000 K in temperature. The critical point was estimated through a bootstrap analysis of a collection of DFT-MD isotherms above and below the critical point. Additionally, we describe the structure and composition of the liquid and vapor around the critical point. Finally, we discuss melting behavior at P=1 bar.

[1]This work was supported by the Z Fundamental Science Program (ZFSP) at Sandia National Laboratories. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

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Date submitted: 19 Mar 2019 Electronic form version 1.4