Abstract Submitted
for the SHOCK11 Meeting of
The American Physical Society

Diffusion Monte Carlo calculations of Xenon and Krypton at High Pressure LUKE SHULENBURGER, THOMAS R. MATTSSON, Sandia National Laboratories — Ab initio calculations based on density functional theory (DFT) have proven a valuable tool in understanding the properties of materials at extreme conditions. However, there are entire classes of materials where the current limitations of DFT cast doubt upon the predictive power of the method. These include so called strongly correlated systems and materials where van der Waals forces are important. Diffusion Monte Carlo (DMC) can treat materials with a different class of approximations that have generally proven to be more accurate. The use of DMC together with DFT may therefore improve the predictive capability of the ab initio calculation of materials at extreme conditions. We present two examples of this approach. In the first we use DMC total energies to address the discrepancy between DFT and diamond anvil cell melt curves of Xe.[1] In the second, DMC is used to address the choice of density functional used in calculations of the Kr hugoniot.

Sandia National Laboratories is a multiprogram laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under Contract No. DE-AC04-94AL85000.

[1]Belonoshko el al. PRB **74**, 054114 (2006)

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Date submitted: 18 Feb 2011 Electronic form version 1.4