Abstract Submitted
for the SHOCK05 Meeting of
The American Physical Society

Designing Meaningful Density Functional Theory Calculations in Materials Science A.E. MATTSSON, P.A. SCHULTZ, M.P. DESJARLAIS, T.R. MATTSSON, K. LEUNG, Sandia National Laboratories — Density functional theory (DFT) methods for calculating the quantum mechanical ground states of condensed matter systems are now a common and significant component of materials research. These methods are also increasingly used in Equation of State work, in particular in the warm dense matter regime. The growing importance of DFT reflects the development of sufficiently accurate functionals, efficient algorithms, and continuing improvements in computing capabilities. As the materials problems to which DFT is applied have become large and complex, so have the sets of calculations necessary to investigate a given problem. Highly versatile, powerful codes exist to serve the practitioner, but designing useful simulations is a complicated task, involving intricate manipulation of many variables, with many pitfalls for the unwary and the inexperienced. We give an overview of DFT and discuss several of the most important issues that go into designing a meaningful DFT calculation. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under Contract DE-AC04-94AL85000.

Ann Mattsson
Sandia National Laboratories

Date submitted: 11 Apr 2005 Electronic form version 1.4