

Abstract Submitted
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Achieving accuracy in first-principles calculations for EOS: basis completeness at high temperatures JOHN M. WILLS, Los Alamos National Laboratory, ANN E. MATTSSON, Sandia National Laboratories — First-principles electronic structure calculations can provide EOS data in regimes of pressure and temperature where accurate experimental data is difficult or impossible to obtain. This lack, however, also precludes validation of calculations in those regimes. Factors that influence the accuracy of first-principles data include (1) theoretical approximations and (2) computational approximations used in implementing and solving the underlying equations. In the first category are the approximate exchange/correlation functionals and approximate wave equations approximating the Dirac equation; in the second are basis completeness, series convergence, and truncation errors. We are using two rather different electronic structure methods (VASP and RSPt) to make definitive the requirements for accuracy of the second type, common to both. In this talk, we discuss requirements for converged calculation at high temperature and moderated pressure. At convergence we show that both methods give identical results. Sandia National Laboratories is a multi-program 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 DE-AC04-94AL85000.

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