Abstract Submitted
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Achieving accuracy in first-principles calculations at extreme temperature and pressure ANN E. MATTSSON, Sandia National Labs, JOHN M. WILLS, Los Alamos National Laboratory — First-principles calculations are increasingly used to provide EOS data at pressures and temperatures where experimental data is difficult or impossible to obtain. The lack of experimental data, however, also precludes validation of the calculations in those regimes. Factors influencing the accuracy of first-principles data include theoretical approximations, and computational approximations used in implementing and solving the underlying equations. The first category includes approximate exchange-correlation functionals and wave equations simplifying the Dirac equation. In the second category are, e.g., basis completeness and pseudo-potentials. While the first category is extremely hard to assess without experimental data, inaccuracies of the second type should be well controlled. We are using two rather different electronic structure methods (VASP and RSPt) to make explicit the requirements for accuracy of the second type. We will discuss the VASP Projector Augmented Wave potentials, with examples for Li and Mo. 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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