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Calculating cold curves for Equation of State using different types of Density Functional Theory codes ANN E. MATTSSON, KYLE R. COCHRANE, JOHN H. CARPENTER, MICHAEL P. DESJARLAIS, Sandia National Laboratories, Albuquerque NM 87185 — With fast computers and improved radiation-hydrodynamics simulation techniques, increasingly complex high energy-density physics systems are investigated by modeling and simulation efforts, putting unprecedented strain on the underlying Equation of State (EOS) modeling. EOS models that have been adequate in the past can fail in unexpected ways. With the aim of improving the EOS, models are often fitted to calculated data in parts of the parameter space where little or no experimental data is available. One example is the compression part of the cold curve. We show that care needs to be taken in using Density Functional Theory (DFT) codes. While being perfectly adequate for calculations in many parts of the parameter space, approximations inherent to pseudo-potential codes can limit their applicability for large compressions. 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.

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