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A Four Phase DFT Based Aluminum Equation of State SCOTT CROCKETT, TRAVIS SJOSTROM, SVEN RUDIN, Los Alamos National Laboratory — We present a description of how density functional theory calculations are utilized as a constraint to basic equation of state modeling in order to generate accurate multiphase equation of state. Three solid phases (fcc, hcp, bcc) and a fluid phase are combined to generated an aluminum equation of state. Density functional calculations of the cold curves and phonons were performed for the solid phases. Quantum molecular dynamic calculations where used for the fluid region. We show comparisons of the ab initio work validated against experiment.

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