

Abstract Submitted
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Properties of Ar at Extreme Compression CARL GREEFF, Los Alamos National Laboratory — I will discuss results from DFT calculations on the equation of state of Ar. These include static lattice, phonon, and first principles molecular dynamics calculations on solid and liquid phases. The calculations extend beyond the metallization transition, which is thought to occur near 500 GPa. Metallization leads to, at most, weak anomalies in the EOS. Various measures of the Grüneisen parameter, γ , are compared. It is found that γ decreases rapidly under compression, and reaches values less than 1/2 at the highest densities. The high pressure melting curve will be discussed.

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