Abstract Submitted
for the SHOCK05 Meeting of
The American Physical Society

***Ab initio* calculations of principal and release isentropes for aluminum**[1] MICHAEL P. DESJARLAIS, MARCUS D. KNUDSON, Pulsed Power Sciences Center, Sandia National Laboratories — We present a direct first-principles approach to calculating isentropes using quantum molecular dynamics (QMD) simulations with density functional theory. The results are compared to several popular EOS models for aluminum as well as principal isentrope and release data from several sources. The agreement with data for aluminum is very good, as is agreement with aluminum data on the principal Hugoniot up to 1200 GPa. We find that our QMD isentropes and Hugoniot for aluminum represent a better overall match to available data than any of the existing aluminum equations of state. We have employed these methods to perform *ab initio* impedance matching calculations for aluminum flyer plates impacting a deuterium sample.

[1]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 No. DE-AC04-94AL85000.

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Date submitted: 07 Apr 2005 Electronic form version 1.4