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**Density functional theory simulations of polyethylene: principal Hugoniot, specific heats, compression and release isentropes**[1] K.R. COCHRANE, Ktech Corp. Albuquerque, NM 87123., M.P. DESJARLAIS, T.R. MATTSSON, Sandia National Laboratories, Albuquerque, NM 87185. — An accurate equation of state (EOS) for polyethylene is required in order to model high energy density experiments for $CH_2$ densities above 1 g/cc, temperatures above 1 eV, and pressures above 1 Mbar. Density Functional Theory (DFT) based molecular dynamics has been established as a method capable of yielding high fidelity results for many materials at a wide range of pressures and temperatures and has recently been applied to complex polymers such as polyethylene [1]. Using high density polyethylene as the reference state, we compute the principal Hugoniot to 350 GPa, compression isentrope, and several release isentropes from states on the principal Hugoniot. We also calculate the specific heat and the dissociation along the Hugoniot. Our simulation results are validated by comparing to experimental data and then used to construct a wide range EOS. [1] T.R. Mattsson et al. Phys. Rev. B **81**, 054103 (2010).

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Thomas R. Mattsson
Sandia National Laboratories, Albuquerque NM 87185.

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