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Predicting the crystalline and porous equations of state for secondary explosives RYAN WIXOM, DAVID DAMM, Sandia National Laboratories — Accurate simulations of energetic material response necessitate accurate unreacted equations of state at pressures much higher than even the C-J state. Unfortunately, for reactive materials, experimental data at high pressures may be unattainable, and extrapolation from low-pressure data results in unacceptable uncertainty. In addition to being low-pressure, the available data is typically limited to the porous state. The fully-dense, or crystalline, equation of state is required for building mesoscale simulations of the dynamic response of energetic materials. We have used quantum molecular dynamics to predict the Hugoniots and 300K isotherms of crystalline PETN, HNS, CL-20 and TATB up to pressures not attainable in experiments. The porous Hugoniots for these materials were then analytically obtained and are validated by comparison with available data. Our calculations for TATB confirm the presence of a kink in the Hugoniot, and the softening of the shock response is explained in terms of a change in molecular conformation and the loss of aromaticity.

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