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Computed Ranking-Hugoniot relations for hexanitrostilbene and hexanitrohexaazaisowurtzitane via density functional theory based molecular dynamics RYAN WIXOM, ANN MATTSSON, THOMAS MATTS-SON, Sandia National Laboratories — Density Functional Theory (DFT) has become an in-dispensable tool for understanding the behavior of matter under extreme conditions, for example confirming experimental findings into the TPa regime and amending experimental data for constructing wide-range equations of state (EOS). The ability to perform high-fidelity calculations is even more important for cases where experiments are impossible to perform, dangerous, and/or prohibitively expensive. We will present computed shock properties for hexanitrostilbene and hexanitrohexaazaisowurtzitane, making comparisons with experimental shock data or diamond anvil cell data, where available. Credibility of the results and proposed methods for validation will be discussed.

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