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Rankine-Hugoniot relationships for molecular crystal explosives calculated using density functional theory based molecular dynamics ANN E. MATTSSON, RYAN R. WIXOM, THOMAS R. MATTSSON, Sandia National Laboratories — Density Functional Theory (DFT) has become a crucial tool for understanding the behavior of matter. The ability to perform high-fidelity calculations is most important for cases where experiments are impossible, dangerous, and/or prohibitively expensive to perform. For molecular crystals, successful use of DFT has been hampered by an inability to correctly describe the van der Waals' dominated equilibrium state. We have explored a way of bypassing this problem by using the Armiento-Mattsson 2005 (AM05) exchange-correlation functional. This functional is highly accurate for a wide range of solids, in particular in compression. Another advantage is that AM05 does not include any van der Waals' attraction. We will demonstrate the method on the PETN Hugoniot, and discuss our confidence in the results and ongoing research aimed at improvement. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

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