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DFT modeling of chemistry on the Z machine

THOMAS R. MATTSSON, Sandia National Laboratories

Density Functional Theory (DFT) has proven remarkably accurate in predicting properties of matter under shock compression for a wide-range of elements and compounds: from hydrogen to xenon via water. Materials where chemistry plays a role are of particular interest for many applications. For example the deep interiors of Neptune, Uranus, and hundreds of similar exoplanets are composed of molecular ices of carbon, hydrogen, oxygen, and nitrogen at pressures of several hundred GPa and temperatures of many thousand Kelvin. High-quality thermophysical experimental data and high-fidelity simulations including chemical reaction are necessary to constrain planetary models over a large range of conditions. As examples of where chemical reactions are important, and demonstration of the high fidelity possible for these both structurally and chemically complex systems, we will discuss shock- and re-shock of liquid carbon dioxide (CO2) in the range 100 to 800 GPa, shock compression of the hydrocarbon polymers polyethylene (PE) and poly(4-methyl-1-pentene) (PMP), and finally simulations of shock compression of glow discharge polymer (GDP) including the effects of doping with germanium. Experimental results from Sandia's Z machine have time and again validated the DFT simulations at extreme conditions and the combination of experiment and DFT provide reliable data for evaluating existing and constructing future wide-range equations of state models for molecular compounds like CO2 and polymers like PE, PMP, and GDP. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Company, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.