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Molecular systems under shock compression into the dense plasma regime: carbon dioxide and hydrocarbon polymers THOMAS R. MATTSSON, KYLE R. COCHRANE, SETH ROOT, JOHN H. CARPENTER, Sandia National Laboratories — Density Functional Theory (DFT) has proven remarkably accurate in predicting properties of matter under shock compression into the dense plasma regime. Materials where chemistry plays a role are of interest for many applications, including planetary science and inertial confinement fusion (ICF). As examples of systems 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 [1] and shock compression of hydrocarbon polymers, including GDP (glow discharge polymer) which is used as an ablator in laser ICF experiments. Experimental results from Sandia's Z machine validate 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. Sandia National Laboratories is a multiprogram 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.

[1] S. Root et. al Phys. Rev. B **87**, 224102 (2013)

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