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Density Functional Theory (DFT) simulations of CO2 under shock compression and design of liquid CO2 experiments on Z[1] T. R. MATTSSON, L. SHULENBURGER, S. ROOT, Sandia National Laboratories, Albuquerque, NM., K. R. COCHRANE, Ktech Corporation, Albuquerque, NM. — Quantitative knowledge of the thermo-physical properties of CO2 at high pressure is required to confidently model the structure of gas-giants like Neptune and Uranus and the deep carbon cycle of the earth. DFT based molecular dynamics has been established as a method capable of yielding high fidelity results for many materials, including shocked gases, at high pressure and temperature. We predict the principal Hugoniot for liquid CO2 up to 500GPa. Our simulations also show that the plateau in shock pressure identified by Nellis and co-workers [1] is the result of dissociation. At low temperatures we validate the DFT results by comparing with diffusion Monte Carlo calculations. This allows for a more accurate determination of the initial conditions for the shock experiments. We also describe the design of upcoming flyer-plate experiments on the Z-machine aimed at providing high-precision shock compression data for CO2 between 150 and 600 GPa. [1] W. Nellis, et. al. , J. Chem. Phys. **95**, 5268 (1991).

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