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First-Principles Equation of State and Shock Compression of Warm Dense Aluminum and Hydrocarbons[1] KEVIN DRIVER, FRANCOIS SOUBIRAN, SHUAI ZHANG, BURKHARD MILITZER, Univ. California, Berkeley — Theoretical studies of warm dense plasmas are a key component of progress in fusion science, defense science, and astrophysics programs. Path integral Monte Carlo (PIMC) and density functional theory molecular dynamics (DFT-MD), two state-of-the-art, first-principles, electronic-structure simulation methods, provide a consistent description of plasmas over a wide range of density and temperature conditions. Here, we combine high-temperature PIMC data with lower-temperature DFT-MD data to compute coherent equations of state (EOS) for aluminum and hydrocarbon plasmas. Subsequently, we derive shock Hugoniot curves from these EOSs and extract the temperature-density evolution of plasma structure and ionization behavior from pair-correlation function analyses. Since PIMC and DFT-MD accurately treat effects of atomic shell structure, we find compression maxima along Hugoniot curves attributed to K-shell and L-shell ionization, which provide a benchmark for widely-used EOS tables, such as SESAME and LEOS, and more efficient models. LLNL-ABS-734424. Funding provided by the DOE (DE-SC0010517) and in part under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. Computational resources provided by Blue Waters (NSF ACI1640776) and NERSC.

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