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Path Integral Monte Carlo Simulations of Warm Dense Plasmas with mid-Z Elements[1] KEVIN DRIVER, FRANCOIS SOUBIRAN, SHUAI ZHANG, BURKHARD MILITZER, University of California, Berkeley — Theoretical studies of warm dense plasmas are crucial for improving our knowledge of giant planets, astrophysics, shock physics, and new plasma energy technologies, such as inertial confined fusion. Path integral Monte Carlo (PIMC) and density functional theory molecular dynamics (DFT-MD) provide consistent, first-principles descriptions of warm, dense matter over a wide range of density and temperature conditions. Here, we report simulation results for a variety of first- and second-row elements. DFT-MD algorithms are well-suited for low temperatures, while PIMC has been restricted to relatively high temperatures due to the free-particle approximation of the nodal surface. For heavier, second-row elements, we have developed a new, localized nodal surface, which allows us to treat bound states within the PIMC formalism. By combining PIMC and DFT-MD pressures and internal energies, we produce a coherent, first-principles equation of state, bridging the entire warm dense matter regime. Pair-correlation functions and the density of electronic states reveal an evolving plasma structure. The degree of ionization is affected by both temperature and density. Finally, shock Hugoniot curves show an increase in compression as the first and second shells are ionized.

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