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First-principles Equations of State and Shock Hugoniots of First- and Second-Row Plasmas[1] KEVIN DRIVER, FRANCOIS SOUBIRAN, SHUAI ZHANG, BURKHARD MILITZER, University of California, Berkeley — A first-principles methodology for studying high energy density physics and warm dense matter is important for the stewardship of plasma science and guiding inertial confinement fusion experiments. In order to address this challenge, we have been developing the capability of path integral Monte Carlo (PIMC) for studying dense plasmas comprised of increasingly heavy elements, including nitrogen, oxygen (J. Chem. Phys., 164507 (2015)), and neon (Phys. Rev. B, 91, 045103 (2015)). In recent work, we have extended PIMC methodology beyond the free-particle node approximation by implementing localized nodal surfaces capable of describing bound plasma states in second-row elements, such as silicon (Phys. Rev. Lett. 115, 176403 (2015)). We combine results from PIMC with results from density functional theory molecular dynamics (DFT-MD) calculations to produce a coherent equation of state that bridges the entire WDM regime. Analysis of pair-correlation functions and the electronic density of states reveals an evolving plasma structure and ionization process that is driven by temperature and pressure. We also compute shock Hugoniot curves for a wide range of initial densities, which generally reveal an increase in compression as the second and first shells are ionized.

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