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First-principles study of equation of state and shock compression of warm dense sodium and other low-Z materials[1] SHUAI ZHANG, KEVIN DRIVER, FRANOIS SOUBIRAN, BURKHARD MILITZER, Univ of California - Berkeley — At high pressure, sodium exhibits exotic properties that deviate from a simple metal. Knowledge of its equation of state (EOS) under simultaneous high pressures and temperatures are still scarce. Following our recent work on hot, dense silicon (Militzer and Driver, PRL 115 (2015) 176403), here we investigate various nodal surfaces in path integral Monte Carlo (PIMC) and reconfirm that localized, Hartree-Fock orbitals yield accurate pressures and internal energies for hot, dense sodium. We combine PIMC and density functional theory molecular dynamics (DFT-MD) in order to derive a coherent, first-principles EOS for sodium over a wide range of densities (1.93-11.60 g/cmˆ3) and temperatures (10ˆ4-1.29x10ˆ9 K). The EOS allows us to study sodium under shock compression. Fully including the electron shell and excitation information, our first-principles EOS predicts the shock Hugoniot curve to have two compression maxima: one below and one above 10ˆ6 K corresponding to the ionization of L and K shell electrons. In this regard our predictions differ from empirical EOS database (SESAME and LEOS), which show only a single peak in compression. Results for other low-Z materials will also be presented. We predict sodium to have an unusually high compression ratio along the principal Hugoniot curve.

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