Path Integral Monte Carlo and Density Functional Molecular Dynamics Simulations of Warm Dense Plastic, Oxygen, Sodium, and Aluminum

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Theoretical studies of warm dense matter and plasmas are a key to improving our knowledge of astrophysical objects - such as stars, white dwarfs and planets - shock physics and new plasma energy technologies - such as inertial confinement fusion. Recent developments in path integral Monte Carlo (PIMC) allowed to study heavier elements and to reach lower temperatures by improving the Fermion nodal structure. Combined with density functional theory molecular dynamics (DFT-MD) it is now possible to derive accurate equations of state and electronic structure properties for a variety of materials over a wide range of pressure-temperature conditions. Here we report our results for a set of CH-plastic materials, oxygen, sodium, and aluminum. We derive the equation of state, the pair-correlation function, the electronic density of states and the shock Hugoniot curves. We analyze the ionization of L and K shell electrons as well as relativistic and radiation effects. We conclude by discussing common trends and differences between the materials under consideration.