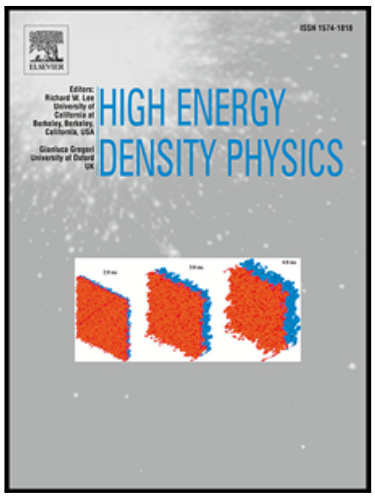

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Comparison of Path Integral Monte Carlo Simulations of Helium, Carbon, Nitrogen, Oxygen, Water, Neon, and Silicon Plasmas

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Abstract

We have performed all-electron path integral Monte Carlo (PIMC) and density functional theory molecular dynamics (DFT-MD) calculations to explore properties of first- and second-row materials in the liquid, warm dense matter, and plasma regimes. Our simulations have covered a wide density-temperature range of roughly $1-15\,\mathrm{g\,cm^{-3}}$ and 10^4-10^9 K). We first analyze the ionization behavior of carbon and water plasma. Then we provide a comparative analysis of the pair-correlation functions and Hugoniot curves of He, C, N, O, Ne, and Si plasmas. Pair-correlation functions give insight into the evolution of plasma structure and ionization processes that are driven by changes in temperature and density. Finally, we show that the maximum shock compression of a material is controlled by the ionization of L-shell and K-shell electrons and depends strongly on this as a function of the atomic number of the material.

Keywords: Path Integral Monte Carlo, Warm Dense Matter, Pair-correlation, Shock Hugoniot

1. Introduction

A rigorous and consistent theoretical description of materials residing in the high energy density physics (HEDP) and warm dense matter (WDM) regimes has been identified [1, 2, 3] as a central goal to the development of key plasma technologies, such as inertial and magnetically confined fusion, shock physics, high energy astrophysics, and stockpile stewardship. Some of the most important pieces of information theoretical calculations can provide include the equation of state (EOS), pair-correlation functions, and transport and optical properties. These quantities provide fundamental information from which many other physical properties can be derived and, subsequently, used to build theoretical models and design HEDP experiments. For example, the design of a fusion experiment [4] relies heavily on understanding how plasma constituents evolve with temperature and density in order to optimize ignition parameters. In addition, knowledge of the plasma dependence on temperature and density provides key constraints on input parameters in hydrodynamic simulations, which are critical in the designs of experiments.

Development of a comprehensive first-principles framework that can accurately and reliably predict plasma properties across the entire WDM regime remains a significant challenge. While semi-analytic plasma models [5] are sufficient for describing weak-to-moderate coupling regimes, first-principles-based methods, such as path integral Monte Carlo (PIMC) [6], orbital-free density functional theory (OF-DFT) [7, 8, 9], and average-atom methods [10, 11, 12], are needed to accurately address the strong coupling regimes along the pathway to fusion. In the WDM regime, materials are only partially ionized, and electrons are still strongly correlated such that quantum effects (quantum degeneracy, ionization, and dissociation) are all relevant for determining plasma properties [13].

PIMC is uniquely suited to provide benchmark-quality predictions in the WDM regime, because it is the only method which is able to treat all of the quantum effects appropriately by solving the full finite-temperature quantum many-body problem. The challenge in PIMC is to further develop the technique for simulations of heavier elements, which we have been working towards for the past several years. We have successively applied PIMC to study progressively higher Z materials in the liquid-, warm-, and plasma regimes, namely hydrogen [14], helium [15], carbon [16], nitrogen [17], water [16], oxygen [18], neon [19], sodium [20] and silicon [21]. As part of this work, we have significantly developed the capability of PIMC to utilize nodal surfaces beyond that of free-particles, which will pave the way for PIMC simulations of heavy elements in the WDM regime. For these materials, we have also performed Kohn-Sham DFT-MD simulations at lower temperatures where most electrons reside in bound states in order to provide one coherent EOS table that covers a wide range of temperature and density conditions.

In this paper, we provide additional analyses of previously published PIMC simulations on low-Z elements. In Section 2, we briefly summarize the details of the simulation methods. In Section 3, we present pair-correlation data from our simulations of carbon and water plasmas.

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