Path Integral Monte Carlo Simulations of Warm Dense Matter

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The properties of materials at extreme pressure and temperature conditions are important in astrophysics and fusion science. When models for Jupiter's interior are constructed to match gravity data from the NASA mission Juno, an accurate knowledge of the equation of state of hydrogen-helium mixtures is essential. Modern dynamic high pressure experiments typically probe megabar and gigabar pressures. In order to provide a comprehensive first-principles description of materials at such extreme conditions, we present results from path integral Monte Carlo simulations. The electrons are treated as fermions while the nuclei behave classically at the high temperatures under consideration. We present equation of state results for first-row elements including carbon, CH plastic, oxygen, water, nitrogen, and neon that we derived with restricted path calculations that relied on free-particle nodes. We compute shock Hugoniot curves and compare with experimental results. We describe how bound states can be incorporated efficiently into the nodal structure (Phys. Rev. Lett. 115:176403, 2015), which enabled us to simulate heavier elements including sodium and silicon.

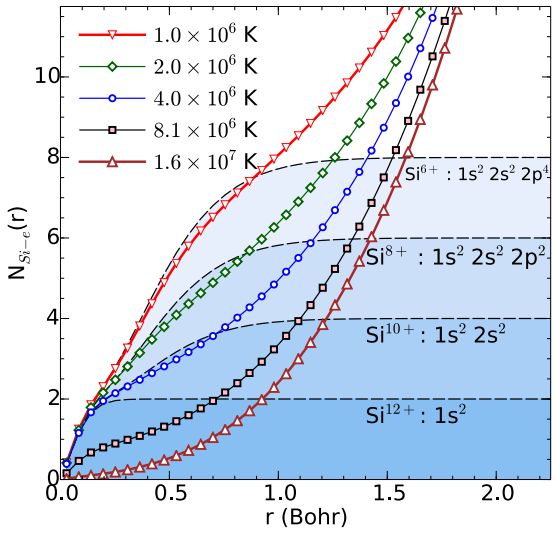

Figure: PIMC predictions for the nucleus-electron correlation functions (symbols) in a hot, dense silicon are compared with isolated ions of various charge states (dashed lines) in order to estimate the degree of ionization for different temperatures.