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All-Electron Path Integral Simulations of Warm Dense Matter: Application to Water and Carbon

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We develop an all-electron path integral Monte Carlo method with free-particle nodes for warm dense matter and apply it to water and carbon plasmas. We thereby extend path integral Monte Carlo studies beyond hydrogen and helium to elements with core electrons. Path integral Monte Carlo results for pressures, internal energies, and pair-correlation functions compare well with density functional theory molecular dynamics at lower temperatures of (2.5-7.5)×105 K, and both methods together form a coherent equation of state over a density-temperature range of 3-12 g/cm3 and 102-109 K. This work appears in Phys. Rev. Lett. 108, 115502 (2012).

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