Abstract Submitted
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All-Electron Path Integral Simulations of Warm, Dense Matter: Application to Water and Carbon[1] KEVIN DRIVER, Department of Earth and Planetary Science, University of California, Berkeley, CA 94720, USA, BURKHARD MILITZER, Department of Earth and Planetary Science and Department of Astronomy, University of California, Berkeley, CA 94720, USA — We develop an all-electron path integral Monte Carlo (PIMC) method for warm dense matter and apply it to study water and carbon. PIMC pressures, internal energies, and pair-correlation functions compare well with density functional theory molecular dynamics (DFT-MD) at lower temperatures and enable the construction of a coherent equation of state over a density-temperature range of 3–12 g/cm^3 and 10^2–10^9 K. PIMC results converge to the Debye-Huckel limiting law at high-temperatures and illuminate the breakdown of DFT pseudopotentials due to core excitations.

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