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Path Integral Monte Carlo Simulations of Warm Dense Matter[1]

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In this presentation, we will give a review of path integral Monte Carlo (PIMC) simulations of warm dense matter. First we discuss earlier work on hot, dense hydrogen and helium. Then we present equation of state results for first-row elements including carbon, CH plastic, oxygen, water, nitrogen, and neon that were 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 ("Development of Path Integral Monte Carlo Simulations with Localized Nodal Surfaces for Second-Row Elements", 115:176403, 2015), which enabled us to extend the applicability range of PIMC computations to lower temperatures and to heavier elements including sodium and silicon. We compare our PIMC-derived equation of state and plasma structure with results from Kohn-Sham and orbital-free density functional calculations. We conclude by discussing how yet heavier elements can be studied with PIMC and how additional properties can be calculated. This work was funded by the DOE (DE-SC0010517, DE-SC0016248).

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