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Classical and quantum simulations of warm dense carbon HEATHER WHITLEY, Lawrence Livermore National Laboratory, DAVID SANCHEZ[1], UC San Diego, SEBASTIEN HAMEL, ALFREDO CORREA, LORIN BENEDICT, Lawrence Livermore National Laboratory — We have applied classical and DFT-based molecular dynamics (MD) simulations to study the equation of state of carbon in the warm dense matter regime (ρ = 3.7 g/cc, 0.86 eV <T <100 eV). We utilize two different classical inter-atomic potentials: 1. LCBOP, designed to simulate solid phases of C, and 2. linearly screened Coulomb (Yukawa) potentials. We observe that LCBOP over-predicts the pair correlations in liquid-C in this regime when compared to the DFT-MD results. Conversely, the Yukawa model seems to produce the correct qualitative features in the static ionic pair distributions at the highest-T, but does not capture the correct correlations at lower T. However, both interaction potentials predict that the decay in the ionic contribution of the specific heat as T approaches infinity is much slower than that predicted by a model based on DFT-MD. These differences in the MD-derived equations of state in warm dense regimes could have important consequences when using classical inter-ionic forces such as these in large-scale MD simulations aimed at studying processes of relevance to inertial confinement fusion. This study points to a need for better interatomic potentials to describe warm dense matter. Prepared by LLNL under Contract DE-AC52-07NA27344.

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