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Warm dense iron equation of state from quantum molecular dynamics TRAVIS SJOSTROM, SCOTT CROCKETT, Los Alamos National Laboratory — Through quantum molecular dynamics (QMD), utilizing both Kohn-Sham (orbital-based) and orbital-free density functional theory, we calculate the equation of state of warm dense iron in the density range 7-30 g/cm^3 and temperatures from 1 to 100 eV. A critical examination of the iron pseudopotential is made, from which we find the previous QMD calculations of Wang *et al.* [Phys. Rev. E 89, 023101 (2014)] to be in error. Our results also significantly extend the ranges of density and temperature which are attempted in that prior work. We calculate the shock Hugoniot and find very good agreement with experimental results to pressures over 20 TPa. Additionally we have utilized the QMD results to generate a new SESAME tabular equation of state for fluid iron, accurate in the warm dense matter region, and also extending to much broader regions of density and temperature than can be accessed by the QMD alone.

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