Dynamic electron-ion collisions and non-local effects on the structures of warm dense matter

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ABSTRACT.

The structural, thermodynamic and transport properties of warm dense matter (WDM) are crucial to the fields of astrophysics and planet science, as well as inertial confinement fusion. WDM refers to the states of matter in a regime of temperature and density between cold condensed matter and hot ideal plasmas, where the density is from near-solid up to ten times solid density, and the temperature between 0.1 and 100 eV. In the WDM regime, matter exhibits moderately or strongly coupled, partially degenerate properties. Therefore, the methods used to deal with condensed matter and isolated atoms need to be properly validated for WDM. It is therefore a big challenge to understand WDM within a unified theoretical description with reliable accuracy. Here, we review the progress in the theoretical study of WDM with state-of-the-art simulations, i.e. quantum Langevin molecular dynamics and first principles path integral molecular dynamics. We study the electronic, ionic structures of warm dense matter from H to Fe, and comparing the equation of states from shock-compressed experiments. Also, we discuss the non-local effects such as van der Waals interactions and nuclear quantum effects on the equation of states and the phase transition of dense hydrogen, showing the consistent results with quantum Monte Carlo method. Finally, the method of calculating electrical conductivity directly from electron molecular dynamics will be shown and the effect of electron-ion collisions could be discussed, which will reduce the conductivity in warm and hot dense matter.

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