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Electron-ion coupled dynamics and structures in warm dense plasmas

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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 firstly show 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, we show the electron-ion relaxation in warm dense hydrogen using Constrained electron force field (CEFF) molecular dynamics. In CEFF, quantum collisions are included since the electrons are treated as Gaussian wave packets, and the Coulomb Catastrophe in classical MD can be avoided. The results of CEFF show that the temperature relaxation time can be up to 3 times longer than that from current popular models and classical MD. Recently, we used ultrafast laser pump-probe technique to produce warm dense Au and obtain the electron kinetics during the laser-matter interactions.

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