Warm dense matter from first-principles molecular dynamics simulations

Ping Zhang

Institute of Applied Physics and Computational Mathematics, 100088 Beijing, China

Thermodynamic properties of matters under high pressure and high temperature conditions are of crucial importance in condensed matter physics, plasma physics, astrophysics, and inertial confinement fusions etc. Warm dense matters are characterized by strong ionic coupling and partially degenerate electronic states. As a consequence, experimental detections as well as theoretical modeling are of great challenge. In this presentation, we show our systematic theoretical studies of thermodynamic properties of warm dense matters. These include: i) Wide range equation of state for liquid hydrogen/deuterium is ultimately obtained by combining two kinds of density functional theory molecular dynamics simulations, namely, first-principles molecular dynamics (FPMD) simulations and orbital-free molecular dynamics (OFMD) simulations; ii) The electronic transport coefficients have been calculated in the framework of density functional theory. We discuss the change in the Lorenz number, which indicates a transition from strong coupling and degenerate state to moderate coupling and partial degeneracy regime for dense hydrogen, helium plasmas; iii) Furthermore, an extended FPMD (ext-FPMD) method based on Kohn-Sham scheme is proposed to elevate the temperature limit of the FPMD method in the calculation of dense plasmas.

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