

Abstract Submitted
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Ionic structures and transport properties of hot dense W and U plasmas YONG HOU, JIANMIN YUAN, National University of Defense technology — We have combined the average-atom model with the hyper-netted chain approximation (AAHNC) to describe the electronic and ionic structure of uranium and tungsten in the hot dense matter regime. When the electronic structure is described within the average-atom model, the effects of others ions on the electronic structure are considered by the correlation functions. And the ionic structure is calculated though using the hyper-netted chain (HNC) approximation. The ion-ion pair potential is calculated using the modified Gordon-Kim model based on the electronic density distribution in the temperature-depended density functional theory. And electronic and ionic structures are determined self-consistently. On the basis of the ion-ion pair potential, we perform the classical (CMD) and Langevin (LMD) molecular dynamics to simulate the ionic transport properties, such as ionic self-diffusion and shear viscosity coefficients, through the ionic velocity correlation functions. Due that the free electrons become more and more with increasing the plasma temperature, the influence of the electron-ion collisions on the transport properties become more and more important.

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