multi-ion molecular dynamics and ion features of x-ray scattering in the warm dense matter regime

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We perform multi-ion molecular dynamics (MIMD) simulation and apply to calculate the ionic structures and x-ray elastic scattering of different charge-state ions in the warm dense matter regime. Firstly, the method is self-consistently used to calculate electron structures of different charge-state ions in the ionic sphere, in which the ion-sphere radii are determined by the plasma density and their charges. And then the ionic fraction is obtained by solving the Saha equation, taking account of interactions among different charge-state ions in the system, and ion-ion pair potentials are computed by the modified Gordon-Kim method in the framework of the temperature-dependent density functional theory on the basis of the electron structures. Lastly, we perform the MIMD simulation to calculate ion features of x-ray elastic scattering for Al.

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