Wave packet molecular dynamics study of the plasma phase transition in warm dense hydrogen

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Despite the fact that hydrogen is the most prevalent element in the universe, its equation of state at high pressures remains poorly understood and raises some fundamental questions. One of such questions is the nature of the plasma phase transition (PPT) [1,2] at pressures above several hundred GPa, at which, perhaps, it passes into a conducting state. Although a large number of experiments dedicated to this problem have been carried out, there is still no consensus on the PPT location: results from experiments with static and ultrafast dynamic compression differ for more than 150 GPa at 1500 K [3,4].

Properties of the dense hydrogen are intensively investigated by means of atomistic ab initio techiques. Quantum Monte-Carlo methods have already given a lot of highly accuracte results for dense hydrogen plasma. First-principles molecular dynamics (FPMD) based on finite-temperature density functional theory (DFT) is another widely deployed tool. However both techniques have difficulties when trying to step beyond Born–Oppenheimer approximation. The difficulties of FPMD applications to non-equilibrium conditions have been considered recently [5]. In this work, we use the wave packet molecular dynamics (WPMD) as a tool that more adequately captures non-adiabatic and non-equilibrium aspects of PPT and gives us the possibility to study the possible metastable states that correspond to this phase transition [2].

Dealing with warm dense hydrogen, we expect the proximity of the electron terms, which, firstly, allows us to work with classical molecular dynamics, and secondly, under these conditions, the contribution from the Pauli prohibition is small, and therefore we can approximate it with a certain potential for accelerating the calculations. In this work, we use the WPMD-based potential eFF [6], in which the contribution from the Pauli exclusion approximates the contribution from the Pauli energy making the unfavorable finding of electrons on one level. eFF provides the combination of particle dynamics for ions with wave packet dynamics for electrons representing them as floating Gaussians. Unlike the more complex antisymmetrized approaches, interactions between electrons in the eFF are restricted to pairwise components only and the total energy of the system is evaluated as in the classical force field methods.

Computations with eFF are carried out at temperatures 1000-15000 K and pressures 80-300 GPa for densities from 0.3 to 1.5 g/cm^3. The analysis of the ionization and dissociation processes in the vicinity of PPT reveals significant influence of the heating rates on the composition hydrogen plasma and gives us a way to describe its metastable states.

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