Metastable states of warm dense hydrogen

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The first-order fluid–fluid phase transition is observed in warm dense hydrogen in shockwave [1] and diamond anvil cell [2] experiments. However, Z-machine experimental observations [3] confirm only an abrupt insulator-to-metal transition. In [4], the interpretation of the experimental data points to the continuous transition to the conducting state of hydrogen, ruling out even the possible existence of the first-order phase transition in the range studied. The jump of density is reproduced by *ab initio* calculations [3,5,6].
The existence of accompanying metastable states of warm dense hydrogen could be used as a criterion, that the transition is of the first order.
This research focuses on obtaining the metastable states of warm dense hydrogen by means of density functional theory and quantum molecular dynamics. The supercell contains 512 atoms. The exchange correlation functional chosen is PBE. The structure of hydrogen is analyzed by pair-correlation functions (PCFs). To obtain the molecular metastable state, the initial configuration should correspond to the molecular state beforehand. We take coordinates and velocities of ions from the equilibrium states or from the obtained metastable ones. Changing the size of the supercell, it is possible to calculate another density and save the state. We reproduce the metastable branch of the isotherm by consequently changing the supercell volume and relaxing configurations at every new density without the thermostat, since under the influence of it the hydrogen less likely remains metastable.
Two isotherms of 700 and 1000 K are investigated. The pressure and the density of the transition are the same as ones obtained in [5], since the calculation parameters are similar. Although the region of the phase transition strongly depends on temperature, the equilibrium and metastable branches of two molecular phase isotherms are located approximately along one and the same curve. The ionized phase branches fit another curve. The metastable region obtained is 470 and 320 kbar by pressure for 700 and 1000 K respectively; the difference between pressure of the metastable and equilibrium states at the same density is approximately 150 kbar for both isotherms. The PCFs have high first peaks along the metastable branch, that confirms hydrogen saving molecular phase. The main results are as follows: (a) the procedure of modeling of the metastable states is developed, (b) the existence of metastable states points out that the phase transition is a first order transition.
The work is supported by the grant 18-19-00734 of the Russian Science Foundation.

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