METASTABLE STATES AND QUANTUM EFFECTS OF NUCLEI IN WARM DENSE HYDROGEN

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A significant number of studies have been devoted to the influence of nuclear quantum effects (NQE) on the thermodynamic properties of hydrogen-containing systems under high pressures [1, 2]. The use of the path integral approach in combination with density functional theory (DFT) allows for effective calculations of these corrections [3].

In this work, we investigate the impact of nuclear quantum effects on hydrogen fluid in the pressure range of 100–200 GPa, where metastable states (molecular and conducting) are observed [4, 5]. The methodology for path integral molecular dynamics (PIMD) simulations using VASP and PIMD software packages has been developed. Our results confirm the existence of metastable states in the hydrogen fluid, providing clear evidence that the observed transition is a first-order phase transition.

Using the VASP+PIMD framework, we computed isotherms in the temperature range of 700–1500 K. A modeling technique for metastable states was developed and successfully applied to the entire set of investigated isotherms. Based on these calculations, the phase boundary was determined, and metastable regions were identified. The persistence of the molecular phase along the metastable branches is confirmed by high values of the first peaks in the pair radial distribution function. Additionally, the latent heat of the phase transition was estimated based on the entropy jump in the pair correlation function. It is demonstrated that the pressure dependence of electrical conductivity exhibits the presence of metastable branches.

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