Metastable states of fluid hydrogen at high pressures: Influence of nuclear quantum effects

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Currently, there is a considerable amount of works investigating the impact of nuclear quantum effects on the thermodynamic properties of systems containing hydrogen at high pressures [1, 2]. The path integral method, in conjunction with density functional theory, effectively takes into account these corrections [3].
The present work proposes for the first time to investigate the effect of this factor on the existence of metastable states of fluid hydrogen at high pressures (100–200 GPa). The technique of performing the framework of molecular dynamics on path integrals using VASP and PIMD software packages has been developed. Metastable states in the hydrogen fluid have been discovered.
Isotherms have been calculated for the temperature range from 700 to 1500 K. A phase curve and an estimate of the metastable regions have been obtained. An estimate of the heat of the phase transition through the jump in pair entropy has been obtained. The electrical conductivity has been calculated as a function of pressure at 700 K.
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