First-principles study of liquid zirconium by the method of quantum molecular dynamics

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Zirconium is one of the main structural materials for nuclear power plants. In this regard, accurate knowledge of the parameters at which the phase transition occurs is particular importance. However, its properties in the liquid phase are still only approximately known. This is due to the fact that experimental measurements by the electrostatic levitation method are limited to temperatures of 2.5–3 kK, and the complexity of measuring the volume of a liquid drop leads to a significant scatter in the density estimates. Either the interpretation of the experimental results by the method of pulsed heating of conductors is difficult due to the speed and complexity of the occurring physical phenomena.

Thus, it seems that at present the only available theoretical approach that can provide information of the thermophysical properties of a substance in the region of a hot expanded liquid is the first-principle method of quantum molecular dynamics (QMD) based on the electron density functional theory.

In this work, the selection of optimal parameters for subsequent modeling, QMD calculations of a detailed grid of isotherms and isochores for the solid and liquid phases and an estimate of the near-zero isobar of zirconium are carried out. Also, comparison with corresponding experimental data is performed.

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