Ab initio calculations of thermophysical properties of liquid metals in the vicinity of the liquid–gas coexistence curve

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The position of the binodal and critical point on a phase diagram of metals is necessary to know for the creation of adequate equations of state at densities below normal. Moreover, in the near-critical region of metals interesting phenomena have been predicted, in particular, the metal–non-metal transition and the cluster formation. Conventional steady-state or quasi steady-state experimental techniques are generally limited to below 2500 K, while results of the dynamic methods, in particular, on isentropic and isobaric expansion may be difficult to interpret because of the complexity of underlying physical phenomena. Moreover, an experimental measurement of critical parameters of metals is very difficult to carry out owing to extremely high temperatures (higher than 3000 K) and pressures (from kilobars to tens of kilobar). A theoretical calculation of near-critical metallic liquid causes significant difficulties because of the degeneration of the electronic subsystem and strong interaction. Unsurprisingly, that until recently there were no theoretical models able to consistently describe different types of dynamical experiments for metals in the vicinity of the liquid–gas coexistence curve. In this work, we are going to discuss our results of quantum molecular dynamics calculations of thermophysical properties and the estimation of critical parameters of W, Mo, U, and some other metals. The interpretation of available experimental data is also presented. This work has been supported by the Russian Science Foundation (grant No. 20-79-10398).