Quantum molecular dynamics calculations of solid and liquid bismuth in the vicinity of melting

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To date, bismuth is widely used in metallurgy, medicine, electronics, including semiconductor materials and also in nuclear industry. Specifically, it is a component of liquid metal heat carriers in existing and prospective reactors. Currently, there a lack of reliable experimental data on the high-temperature properties of liquid bismuth for temperatures above 2000 K.

Quantum molecular dynamics (QMD) based on the electron density functional theory is a preferred computational method for exploring thermodynamic properties of liquid metals, because it takes into account a complex electronic structure of atoms and it does not use any empirical data except for charges and masses of ions.

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

This work has been supported by the Russian Science Foundation (grant No. 20-79-10398).