Ab initio investigation of liquid sodium thermodynamics in near-critical states

Paramonov M.A.[1,@], **Minakov D.V.**[1,2], **Galtsov I.S.**[1,2], **Onegin A.S.**[1,2] **and Levashov P.R.**[1,2]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow, 125412, Russia
[2] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, 141701, Russia

[@] mikhail-paramon@mail.ru

Liquid metals such as sodium are attractive coolants in the nuclear power industry because their high thermal conductivity and flowability enable efficient heat removal and high heat-transfer rates in power systems. Since sodium is widely used in fast reactors, reliable design and safety analysis of sodium-cooled systems requires accurate thermophysical properties of sodium over broad liquid and near-critical conditions where experiments are limited.

The quantum molecular dynamics (QMD) method is increasingly used to predict the physical properties of materials in temperature ranges where it is difficult to reproduce experimental data or where experiments are completely impractical. The approach combines finite-temperature density functional theory for electrons with classical dynamics of ions and does not depend on any additional empirical data.

The aim of this work is to investigate the thermodynamic and transport properties of sodium in the liquid and near-critical conditions using QMD. We performed simulations on a detailed grid of isotherms and isochores in the liquid phase and in the vicinity of the two-phase boundary. Based on the obtained equation of state, we estimated the critical-point parameters, transport coefficients, including viscosity and thermal conductivity, and derived thermal expansion behaviour. The available relevant experimental data are also analysed and discussed.

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