Investigation of the high-temperature properties of lead in liquid and near-critical states by quantum molecular dynamics

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Lead's unique physical and chemical properties make it indispensable in various industrial applications, particularly in the nuclear power industry, where it is valued for its effectiveness as a coolant and radiation shield in modern reactors due to its high density, excellent corrosion resistance and ability to absorb radiation. And accurate measurement of the critical point parameters and transport properties of lead is of paramount importance to ensure safe and efficient design and operation of nuclear reactors.
The quantum molecular dynamics method is increasingly being used to determine the physical properties of materials in temperature ranges where it is difficult to reproduce experimental data or where experiments are completely impractical. This approach is based on density functional theory and does not depend on any additional empirical data.
The aim of this work is to investigate the thermodynamic and transport properties of lead in the vicinity of the liquid-gas two-phase boundary using the QMD method. QMD calculations of a detailed grid of isotherms and isochores for the liquid phase of lead, estimation of critical parameters, thermal expansion curve, viscosity and thermal conductivityare carried out. The available relevant experimental data is also analysed and discussed.
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