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Thermodynamic properties by equation of state and from Ab initio molecular dynamics of liquid potassium under pressure[1] HUAMING LI, YANTING TIAN, YONGLI SUN, Taiyuan Univ of Technology, MO LI, Georgia Institute of Technology, NONEQUILIBRIUM MATERIALS AND PHYSICS TEAM, COMPUTATIONAL MATERIALS SCIENCE TEAM — In this work, we apply a general equation of state of liquid and Ab initio molecular-dynamics method to study thermodynamic properties in liquid potassium under high pressure. Isothermal bulk modulus and molar volume of molten sodium are calculated within good precision as compared with the experimental data. The calculated internal energy data and the calculated values of isobaric heat capacity of molten potassium show the minimum along the isothermal lines as the previous result obtained in liquid sodium. The expressions for acoustical parameter and nonlinearity parameter are obtained based on thermodynamic relations from the equation of state. Both parameters for liquid potassium are calculated under high pressure along the isothermal lines by using the available thermodynamic data and numeric derivations. Furthermore, Ab initio molecular-dynamics simulations are used to calculate some thermodynamic properties of liquid potassium along the isothermal lines.

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