Structural transformations in liquid selenium under high pressures

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It has long been known that simple liquids undergo a continuous structural transition with changes in temperature or pressure. Research conducted over the past few decades has shown that some simple liquids undergo a discontinuous first-order phase transition, which is accompanied by changes in density, entropy, and structure, and is known as the liquid-liquid phase transition (LLPT). In 1989, Academician V.V. Brazhkin published the article [1], in which a conductivity jump and a volume effect were observed, which suggests that the semiconductor-metal transition is a first-order phase transition. In this work, liquid selenium at high pressures was studied using density functional theory (DFT), machine learning interatomic potentials and molecular dynamics. There were conducted series of calculations along different isotherms, the radial distribution function and the dependences of volume, coordination number and isothermal compressibility on pressure along these isotherms were analyzed. No volume jumps were observed, which indicates the absence of a phase transition of the first order. A minimum is observed on the radial distribution function, which indicates a change in the local structure of the liquid (structural transition). Also there is a kink on the isothermal compressibility, which may be a consequence of a structural transition.

[1] Brazhkin V V, Voloshin R N and Popova S V 1989 *Soviet Journal of Experimental and Theoretical Physics Letters* **50** 424