CALCULATION OF ATOM WORK FUNCTIONS FROM LIQUID INTO GAS WITHIN THE MOLECULAR-KINETIC THEORY

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S u m m a r y

On the basis of model representations, the analysis of the first equation of the Bogolyubov—Born—Green—Kirkwood—Yvon (BBGKY) chain of equations for the equilibrium two-phase dielectric "liquid — gas" system is performed. The asymptotic values of the monatomic potential in liquid and gas are calculated. The expression for an atom work function from liquid to gas is obtained. Model calculations of the atom work function for many dielectric liquids with application of the Lennard—Jones (LJ) potential and the Barker—Henderson (BH) and Weeks—Chandler—Andersen (WCA) models for a radial distribution function along the saturation line from melting temperatures to critical temperatures are performed. Within the framework of model calculations, the effect of the atom density profile near the liquid-gas interface on the atom work function from liquid into gas is analyzed. For comparison, in the first order of thermodynamic perturbation theory, the estimation of the entropy contribution to the liquid-gas phase transition heat is carried out. The relationship between the atom work function and the liquid stability criterion is discussed.