THE KEY THERMODYNAMIC CHARACTERISTICS OF NUCLEATION ON UNCHARGED AND CHARGED PARTICLES WITHIN THE GRADIENT DFT

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Using the gradient density functional theory, we formulated the equations for the molecular density profiles around the uncharged and charged particle in stable and unstable droplets in equilibrium with supersaturated vapor for one-component polar and nonpolar system described by the van der Waals and the Carnaham-Starling models for the bulk liquid and vapor phases and interfaces. Numerical calculations with different chemical potential of condensate have been performed for water and argon droplets. This given a possibility to determine the height of the activation barrier of homogeneous and heterogeneous nucleation as a function of supersaturation under the certain temperature of the system. The particle serving as a condensation center in the case of heterogeneous nucleation has been characterized by an attractive short-range molecular potential and the long-range electric Coulomb potential. The dielectric permittivities of the droplet-vapor systems have been taken as known functions of the local condensate density and temperature for polar and nonpolar fluids. Detailed numerical calculations of the condensate chemical potential in presence of the capillary, electrostatic and molecular forces have been performed for water and argon droplets.