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## Molecular Simulation of Homogeneous Vapor-Liquid Nucleation

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Atmospheric aerosol particles are ubiquitous and have an influence on the Earth's environment by scattering and absorbing solar radiation and affecting cloud formation and precipitation. New particle formation in the atmosphere is a major source of ultrafine aerosol particles and is thought to regulate the number concentrations of cloud condensation nuclei. New particle formation consists of nucleation of small molecular clusters and their subsequent growth. These processes are still poorly understood. Ion-induced nucleation due to atmospheric ions created by cosmic rays and radioactive substances such as radon has been proposed as a mechanism of new particle formation.

Classical nucleation theory, which is based on a simple liquid droplet model, is widely used as a method to describe nucleation processes. There is a considerable discrepancy between nucleation rates estimated by the theory and experimental values. The failure of the theory is thought to be caused by the incorrectness of the liquid droplet model. Nucleation is controlled by small molecular clusters, and it is inappropriate to assume such small clusters as macroscopic droplets.

In this study we conducted simulations of nucleation using the molecular dynamics method and constructed a kinetic model to describe the processes. We additionally calculated thermodynamic properties of ion clusters involved in ion-induced nucleation. The stability of the ion clusters compared to the corresponding neutral clusters will be discussed.

Keywords: Vapor-Liquid Nucleation, Molecular Dynamics Simulation