# Molecular Simulation of Nucleation Phenomena

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Nucleation, the formation of embryos of a new phase from a metastable mother phase, plays a unique role for phase transitions and is an important factor for many industrial and environmental processes. Molecular simulation offers an opportunity to advance molecular-level understanding of nucleation phenomena. However, conventional simulation approaches are hampered by the extremely low probabilities for the occurrence of clusters near the critical nucleus size and the extremely slow transfer of particles between clusters of different sizes. To overcome these problems, a novel simulation approach is developed that integrates aggregation-volume-bias, configurational-bias, and adiabatic-nuclear-electronic-sampling Monte Carlo algorithms with multi-dimensional umbrella sampling and histrogram-reweighting techniques. Applications to the nucleation of neat water, water/ethanol and water/nonane mixtures, and water in the presence of ions are discussed.