

Aggregation-volume-bias Monte Carlo simulations of vapor-liquid nucleation barriers for Lennard-Jonesium

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Abstract

A combination of the aggregation-volume-bias Monte Carlo algorithm and the umbrella sampling technique is applied to investigate homogeneous vapor-liquid nucleation. This combined approach is simple, general, and robust. Its efficiency is demonstrated for nucleation of Lennard-Jonesium, for which the precise calculation of the nucleation barriers takes only a few minutes at higher supersaturations to a few hours at lower supersaturations. Comparison of the simulation results to the classical nucleation theory (CNT) shows that CNT overestimates the barrier heights by a value nearly independent of the supersaturation, but provides a reasonable description of the critical cluster sizes.