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Gas-to-Liquid Nucleation in Atmospherically Relevant Multi-Component Systems

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場 所: 東京大学工学部2号館 3階 31B

Abstract:

Aerosol formation is of prime interest to the nucleation Community due to its effects on atmospheric weather patterns. In our study, we test the applicability of the MC-AVUS algorithm – an Aggregation-Volume-Bias Monte Carlo method combined with Umbrella Sampling, in exploring higher-order multi-component systems. Our past studies had been able to reproduce experimentally observed nucleation behaviors of unary, binary, and ternary systems. From these nucleations, we have demonstrated that thermophysical properties such as surface tension and density can be calculated within reasonable error. Nucleation free energy landscapes can also be derived from our simulations. This, and our ability to probe the atomistic feratures of the critical nuclei, allows us to predict and rationalize mechanistic pathways. Through an improved simulation protocol, we are investigating the homogeneous vapor-to-liquid nucleation of three quaternary systems: (1) a realistic four component WNBA (water / n-nonane / 1-butanol / ammonia) system, (2) a Martian (carbon dioxide /water / methane / argon) atmosphere analog system, and (3) Ar-4 (a hypothetical Argon-like atoms) system. Simulation convergence below cluster sizes of 25×25×25×25 molecules has been achieved for these systems. Existence of nuclear motifs as well as composition-dependent preferences of nucleation pathways have been observed even at small cluster sizes. Insights from this study could help facilitate modeling of complex alien atmospheric nucleation phenomena, understanding of complex mixing patterns, and manipulating micro-emulsions for atmospheric aerosol science-related applications.

主催: 東京大学大学院工学系研究科専攻間横断型教育プログラム 機械システム・イノベーション（GMSI）
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