"Too Small is Never Too Small: Utilizing Advanced Path Sampling Techniques to Probe the Kinetics and Mechanism of Rare Events, From Atmospheric Ice Nucleation to Ion Transport"

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Abstract

More often than not, scientists are challenged with the daunting problem of measuring or computing astronomically small quantities that are related to the occurrence of rare events. A phenomenon is called a rare event when the amount of time that elapses before its occurrence is orders of magnitude longer than the time needed for its completion. Rare events are ubiquitous in nature and span a wide range of phenomena such as earthquakes, telecommunication and power grid failures, protein folding, genetic mutations, and crystallization. Capturing the statistical nature of such events is key in many applications, including materials synthesis, climate modeling, bioengineering and medicine. Unfortunately, achieving this with conventional experiments or simulations is inefficient at best as the waiting times for observing a single rare event can surpass the experimentally or computationally accessible timescales by several orders of magnitude. This becomes an almost impossible undertaking when the rate of occurrence of a rare event is astronomically small. Under such circumstances, specialized sampling techniques are necessary for capturing the statistical features of the corresponding rare event.

This presentation will be dedicated to showcasing our work on characterizing rare events using an advance sampling technique known as forward flux sampling (FFS), alongside a brief discussion of a novel variant of FFS recently developed in my group suited for studying aggregation phenomena such as nucleation. I will, in particular, discuss our application of FFS to probe the kinetics and microscopic mechanism of two scientifically and practically important rare events, namely ice nucleation under atmospherically relevant conditions, and ion and solute transport through semipermeable nanoporous membranes. An emphasis will be put on not only the ability of FFS to characterize their kinetics, but also its power to provide molecular insights into the underlying mechanisms of these processes.

Bio

Professor Amir Haji-Akbari received his B.Sc. in Biotechnology from the University of Tehran, and his Ph.D. in Chemical Engineering from the University of Michigan, Ann Arbor, under the supervision of Professor Sharon Glotzer. After finishing his PhD, he joined Professor Pablo Debenedetti's Group at Princeton University as a postdoctoral researcher. He has been an Assistant Professor of Chemical & Environmental Engineering at Yale since January 2017, and his group develops and utilizes advanced sampling techniques to study rare events in soft matter systems. He has won several awards such as the NSF CAREER Award and the AIChE COMSEF Young Investigator Award.