Casting Light on Things Unseen: Molecular Simulation and Data Visualization

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Attempts to advance scientific understanding and chemical research face fundamental epistemological questions. First, what are the tools for realizing knowledge? Second, how does one's methodological choices (e.g., tools with their own unique capabilities and properties) influence one's perceptions and conclusions? In this talk, I will explore these questions at the interdisciplinary nexus between chemistry and computer science. I will illustrate how computer simulations, specifically molecular dynamics simulations, are powerful tools for probing the molecular-level details of chemical phenomena, and thus realizing chemical insights into disparate processes and materials (e.g., gas hydrates and polymers). In particular, it will be demonstrated that crystallization processes involve funnel-shaped potential energy landscapes akin to those associated with protein folding, and that the nanoscopic characteristics of crystallization processes are more complex than the visions of crystallization afforded by prevailing theories. I will also discuss data visualizations as tools for converting data into chemical insights, and thus changing how one understands and envisions chemical processes. I will illustrate how visualizations can provide new perspectives on chemical datasets while opening up new possibilities both in terms of the types of chemical research questions that one can ask and the ways in which one can address those questions. This talk interweaves computational chemistry and computer science research to advance both molecular-level understanding of ordering processes, and methodological knowledge relevant to realizing chemical knowledge.