



Department of Chemical Engineering presents

Professor Sapna Sarupria



Department of Chemical & Biomolecular Engineering
Clemson University

December 5, 2018 - Goergen Hall 101 @ 3:25pm

"Freezing Water and Aqueous Solutions:

Elucidating the Molecular Ballet Using Computer Simulations"

Nucleation – that is the onset of a new phase from a metastable phase – is a difficult phenomenon to study both experimentally and computationally. Nucleation relevant spatial and temporal resolution is difficult to access in experiments. In contrast, while computer simulations are perfectly suited to probe these length and timescales, sampling statistically relevant number of nucleation events is computationally expensive. In our research, we use advanced sampling techniques in conjunction with molecular dynamics simulations to sample hundreds and thousands of nucleation events. We apply these methods to study heterogeneous ice nucleation and gas hydrate nucleation. Heterogeneous ice nucleation relates to freezing of water driven by the presence of an impurity such as a mineral surface. Interestingly, it is not yet understood what about a surface promotes or inhibits the formation of ice. We use simulations of salt (silver iodide) and mineral (kaolinite) surfaces to provide insights into the properties of a surface that facilitate ice formation. These findings can help design surfaces that either inhibit ice nucleation (for example in cases such as wind mills, power lines, and transportation) or that promote ice nucleation (for example in cases such as food preservation and cryopreservation). Gas hydrates are crystalline (ice-like) solids formed by water forming cages around guest molecules such as methane, carbon dioxide and tetrahydrofuran. These form at low temperatures and high pressure conditions and are a flow assurance problem in the oil and gas industry. In addition, hydrates can be potential energy source, and be used for gas separation and water desalination. The fundamental question that remains unanswered is -- how does the solution of guest and water transform into this crystalline solid. Our simulations provide insights into the mechanisms of hydrate nucleation and highlight its dependence on the water solubility of the guest molecules. These findings will facilitate design of promoters and inhibitors of gas hydrates. Collectively, my talk provides an overview of the intricate behavior of water molecules in transforming from liquid to the solid phase.

Short Biosketch:

Sapna Sarupria is an associate professor in Chemical and Biomolecular Engineering at Clemson University. She received her B. Tech in Chemical Engineering from India in 2002 and her Ph.D. from Rensselaer Polytechnic Institute in 2009. After her PhD, she did her postdoc in Princeton University before joining Clemson University. Dr. Sarupria's research focuses on using molecular modeling and computer simulations for materials engineering. Her research group has several thrust areas including studies of rare events in molecular simulations, phase transitions in water and aqueous solutions, engineering membrane fouling resistant membranes, and design of robust enzymes. She has received several awards including the Doctoral New Investigator award by American Chemical Society Petroleum Research Fund, OpenEye Outstanding Junior Faculty Award by ACS Comp Division, Dean's Faculty Fellow by Clemson College of Engineering and Science and Award of Excellence from Clemson's Board of Trustees. She recently also received the NSF CAREER award.