IOWA STATE UNIVERSITY
DEPARTMENT OF MECHANICAL ENGINEERING

Probing mesoscopic structure-property relationship using all-atom molecular dynamics simulations

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Abstract:
Nanomaterials exhibiting complex multi-property behavior and response have become important in key technological areas including solar conversion, energy storage, efficient electronics, medicine, and sensing. In functional devices employing these nanomaterials, it is critical to identify the structure-functionality correlation for an ensemble of nanoparticles. The factors determining such correlations vary over a wide range of length and time scales (intermolecular interactions at nanoscale to mesoscopic interfacial interactions and particle-particle interactions). This talk will focus on large-scale molecular dynamics simulations involving several million atom systems to probe structure-functionality at the mesoscale as well as mesoscale phenomena that are of importance for materials synthesis and design. The rapid advances in computational power as well as the need to understand the full functionality of new materials with atomistic resolution has led to an exponential growth in the size and complexity of the data used to describe them. Using representative systems ranging from solvated thermo-sensitive polymer relevant to biomedical application to reactive complex oxides and tribological interfaces, this talk will focus on elucidating some key mesoscopic phenomena at material interfaces using multi million-atom atomistic simulations. This talk also highlights some of the computational challenges, the data-intensive nature of these calculations and the limitations of existing force-fields typically employed in molecular simulations. Finally, we will also present some of our on-going efforts on developing accurate reactive-force fields to bridge the gap between electronic structure and classical molecular dynamics simulations and describe such mesoscopic interfaces.

Biography:
Subramanian K. R. S. Sankaranarayanan received his BS degree in Chemical Engineering from Nagpur University, in 2000, and his MS degree in Chemical Engineering from Indian Institute of Science, Bangalore, India, in 2002. After receiving his Ph.D. in Chemical Engineering in 2007 from University of South Florida, Tampa, he was a post-doctoral fellow at Harvard University (2007-2010). Dr. Sankaranarayanan is currently an Assistant Scientist at the Center for Nanoscale Materials at Argonne National Laboratory. His work focuses on development and application of multi-scale models spanning a wide range of spatial and temporal scales (finite element method, kinetic Monte-Carlo, coarse-grained, classical molecular dynamics and density functional theory) to a broad range of problems from electrochemical energy storage, corrosion, tribology and catalysis to chemical and biomedical sensing. He currently is leading an Argonne strategic effort on force-field development for reactive interfaces.