Molecular Understanding of Fluids in Nanochannels: Computational Studies

There is a growing interest in investigating transport and electrochemical phenomena in synthetic membrane nanopores because of the possibility of mimicking selective ion transport found in protein channels in cell membranes of living systems and also towards the development of single molecule detection systems. Several experimental approaches such as the track etch method and the ion beam method have been used with increasing success in recent years to characterize the ionic transport through nanopores of varying diameters. However, fundamental questions regarding the effects of confinement on diffusion and mobility of ions need to be resolved for better design of these nanochannel/nanopore based devices and to propose novel sensing mechanisms based on chemical functionalization. The traditional continuum theory typically used in the analysis of electrochemical phenomena in micro-fluidic channels cannot take into account the effects caused by the finite size of the ions and water and the water accessible volume of the nanopore. This requires atomic scale simulations (e.g. molecular dynamics simulations) where finite size of ions and water is explicitly treated. However, order of the time scales and the length scales possible in atomistic molecular dynamics (MD) simulations is far less than realistic design calculations. Further, it is known that in small diameter nanopores (~ 3nm and less) the wall partial charges and the polarization effects can influence the transport coefficients. These can be computed from Density functional theory (DFT) or by semiempirical methods. In this talk, I will present computational studies towards a molecular understanding of fluids and the development of multiscale methods. A number of results will be presented showing the significance of confinement, surface charge density and partial charges on water and ion transport.

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B02 Coordinated Science Lab

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Professor N. R. Aluru received the B.E. degree with honors and distinction from the Birla Institute of Technology and Science (BITS), Pilani, India, in 1989, the M.S. degree from Rensselaer Polytechnic Institute, Troy, NY, in 1991, and the Ph.D. degree from Stanford University, Stanford, CA, in 1995. He is currently an Associate Professor in the Department of Mechanical and Industrial Engineering at the University of Illinois at Urbana-Champaign (UIUC). He is also affiliated with the Beckman Institute for Advanced Science and Technology, the Department of Electrical and Computer Engineering and the Bioengineering Department at UIUC. He was a Postdoctoral Associate at the Massachusetts Institute of Technology (MIT), Cambridge, from 1995 to 1997. In 1998, he joined the University of Illinois at Urbana-Champaign (UIUC) as an Assistant Professor. Dr. Aluru received the NSF CAREER award and the NCSA faculty fellowship in 1999, the 2001 CMES Distinguished Young Author Award, the 2001 Xerox Award for Faculty Research, and the Willett Faculty Scholar Award in 2002. He is a Subject Editor for the IEEE/ASME JOURNAL OF MICROELECTROMECHANICAL SYSTEMS, Associate Editor for the IEEE TRANSACTIONS ON CIRCUITS AND SYSTEMS II and serves on the Editorial Board of a number of other journals.