

IOWA STATE UNIVERSITY

Center for Multiphase Flow Research and Education

Conformations and equilibrium dynamics of polar polymers in aqueous solution as studied by molecular dynamics simulations

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Abstract

We present our recent work on structure and short range dynamics of aqueous solutions of polar polymers, charged and uncharged, homopolymers and block copolymers using atomistic molecular dynamics simulations. Studies of conformations, intermolecular structure, dynamics and diffusion of polymers and block copolymers, and the aggregation and self-assembly in solution will be presented in this talk.

Biography

Upendra Natarajan received his B.Tech. in Chemical Engineering from Indian Institute of Technology Bombay, M.S. in Chemical Engineering from University of Kansas, Ph.D. in Polymer Science from University of Akron, and did his post-doctoral work at Cornell University. Following this, he worked as Staff Scientist at the National Chemical Laboratory (CSIR, India) Pune. Since 2007 he is at Indian Institute of Technology Madras. His areas of research interests are broadly in the field of Polymer Science and Engineering, in particular molecular modeling and simulations, statistical mechanics and thermodynamics. In specific his current areas include conformations and dynamics of water soluble uncharged and charged polymers, polyelectrolyte block copolymers in aqueous solution, water-alcohol mixtures and glassy polymer phases, where he is interested in intermolecular structure and short-range dynamics. Of particular long-term interests are long-range effects of dynamics in polymer solutions, microscopic and mesoscale modeling of flow behavior and dynamics of semi-dilute and concentrated polymeric solution. His interests also include kinetic theory and to develop mesoscale models of polymer and polymer-particle containing solutions. His course teaching includes undergraduate transport phenomena, interfacial science and engineering, polymeric materials, molecular theory of solutions.

This seminar counts towards the ME 600 seminar requirement for Mechanical Engineering graduate students.

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