ENGINEERING SEMINAR ANNOUNCEMENT

Polymers in Ionic Liquids

Fri, Nov. 17th 11:00 a.m. Engineering B-221



Arun Yethiraj, PhD V. W. Meloche-Bascom Professor of Chemistry Department of Chemistry University of Wisconsin-Madison

This event sponsored by FAMU-FSU Department of Chemical & Biomedical Engineering Arun Yethiraj was born in India and spent most of his childhood in Bombay. He received a B. Tech. in Chemical Engineering from the Indian Institute of Technology, Bombay, in 1985, an M.S. in Chemical Engineering from iana State University in 1987, and a PhD in Chemical Engineering from North Carolina State University in 1991. ofessor Yethiraj has established a research program focused on interdisciplinary research. His theoretical toolbox includes field theories, liquid state theories, quantum chemistry, classical density functional theory, continuum mechanics, Monte Carlo and molecular dynamics simulations, and machine learning methods. He has worked in a diverse set of research areas including polymer surface behavior, colloidal dispersions, polyelectrolyte solutions and coacervates, liquid crystals, surfactants, macromolecular folding, protein self-assembly, membrane biophysics, and battery electrolytes. His research in chemical physics and physical chemistry is

Ionic liquids have generated considerable excitement for their varied potential applications and their interesting physical properties. The viability of ionic liquids (ILs) in materials applications is limited by their lack of mechanical integrity, which may be provided by mixing them with a polymeric material.

This talk focuses on computational studies of PEO in imidazolium ILs. We develop a physically motivated first principles force field for PEO and [BMIM] [BF4]; this force field is in quantitative agreement with experiment with no adjustable parameters. Based on the same quantum calculations we develop a hierarchy of united atom models with decreasing resolution and increasing computational efficiency. Microsecond simulations are required to obtain converged properties of the polymer, which displays a combination of ring-like and extended conformations. We use machine learning methods to establish the phase behavior of these systems.

Professor Yethiraj is an Alfred P. Sloan Research Fellow, has received the NSF CAREER award, and an Alexander von Humboldt Fellowship. In 2020, he received the Chemical Research Society of India Medal. He received the 2022 Award in Theoretical Chemistry. He is a Fellow of the American Physical Society. He served as Senior Editor for The Journal of are Physical Chemistry (2007-2019).