



School of Interdisciplinary Research Indian Institute of Technology Delhi New Delhi



Invites you all to a Seminar on

Polymers in Ionic Liquids

Date & time: September 14, 2022 (Wednesday), 11:00 am
**Venue: Chemistry Department Committee Room- MS710,
6th Floor, Main Building, IIT-Delhi**



Prof. Arun Yethiraj
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Abstract

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.

BRIEF CV

Dr. Arun Yethiraj is a Professor in the University of Wisconsin-Madison, USA. He is awarded doctoral degree in Chemical Engineering from North Carolina State University in the year of 1991. He is one of the highly decorated theoretical researchers in the USA. He has obtained several notable fellowships, including, Samuel C Johnson, Alexander von Humboldt, and American Physical Society to name a few. He is awarded with Vilas Associate award in 2006. He has served as a Senior Editor for the Journal of Physical Chemistry.

Research Interest: His research focuses primarily on computational and theoretical studies of the soft condensed matters. He is more interested in understanding structure-property relationship at atomistic level for the soft matters. His research has two main components: the development of force fields and methods, and the application of these to understand the structure and dynamics of the condensed phases.

