

## **Seminar**

### **Polymers in ionic liquids**

**Arun Yethiraj**

**University of Wisconsin, Madison**

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][BF<sub>4</sub>]; 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 behaviour of these systems.

***Thursday, Jul 7<sup>th</sup> 2022***

***04:00 PM***

***Venue: Auditorium***