

Department of Physics & Astronomy

Dr. Amalie Frischknecht

Sandia National Laboratories

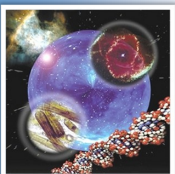
Friday, October 28, 2011

Time: 3:00 p.m. - 4:00 p.m.

BB 3.04.18

Morphologies in Ion-Containing Polymers

Ionomers, polymers containing a small fraction of covalently bound ionic groups, are promising as possible solid electrolytes in batteries. In particular, a single-ion conducting polymer electrolyte would be safer and have higher efficiency than the currently-used liquid electrolytes. However, to date ionomeric materials do not have sufficiently high conductivities for practical application. This is most likely because the ions tend to form aggregates, making counterion diffusion unacceptably slow. A key question is therefore how molecular properties affect the ionic aggregation and ion dynamics. Recent experimental advances have allowed synthesis and extensive characterization of ionomers with a precise, constant spacing of charged groups. Because the molecular architecture is controlled and these materials show increased ionic aggregate ordering versus their randomly spaced analogs, this set of experiments is ideal for direct comparisons with molecular simulations. In this talk, I will first give an overview of the behavior of ionomers and outline some outstanding questions about their structure and dynamics. I will then describe our approach to modeling ionomers with precise spacing between charged groups and give comparisons with experiment. The focus will be on simple coarse-grained models which are designed to capture the basic physics of ion-containing polymer liquids, allowing us to develop an understanding of the relationship between molecular architecture and ionic aggregate morphology.



Department Contact Information

Dr. Marcelo Marucho • 210.458.7862 • Marcelo.Marucho@utsa.eduLaurie De La Paz • 210.458.4425 • Laurie.DeLaPaz@utsa.edu<http://physics.utsa.edu/>