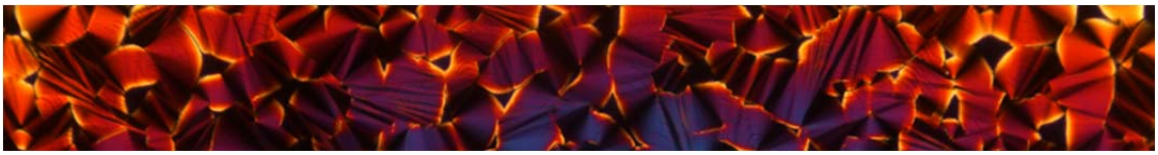

# SOFT MATERIALS RESEARCH CENTER

## SPECIAL SEMINAR SERIES

# A New Picture of Ionomer Melt Structure and Dynamics


**Mark Stevens**

*Sandia National Laboratories, Center for Integrated Nanotechnologies, Albuquerque, New Mexico*



Ionomers are ion-containing polymers that have applications from golf ball covers to battery electrolytes. We have performed both coarse-grained and atomistic molecular dynamics simulations on (dry) ionomer melts with precise spacing of the charged groups. These simulations reveal a new picture of the ionomer morphology and dynamics. In experimental scattering data there is the well-known 'ionomer peak' associated with ionic aggregates. The structure factor calculated from the simulations also has an ionomer peak that shows the same trends as a function of molecular architecture as in experiments. In addition, the simulations directly reveal aggregate structure that has not yet been measured experimentally. Our simulation data shows that the aggregates tend to have a stringy structure with larger scale structure that is strongly dependent on molecular architecture. If the ions are bound pendant to the backbone, then compact, isolated aggregates form, but if the ions are in the backbone, then extended, percolating aggregates form. Our atomistic simulations show that the aggregate structure also depends on the counterion. In addition, we have treated partially neutralized systems with the atomistic simulations and see the effect of hydrogen bonding on the aggregate formation. With the coarse-grained simulations, we have studied the ionomer dynamics. The key mechanism of ion transport for systems with isolated aggregates is collision and merger of the aggregates and exchange of ions upon reformation of the aggregate after the collision. For the percolated systems, the counterions can move throughout the aggregate, and the conductivity is largest for these systems. The simulations have provided a rich new description of these ionomers, which suggest means for improving material properties and opportunities for understanding ion diffusion through random media.


**Wednesday, February 4th at 1:30 p.m. Duane Physics G126**


*Sponsored by the Soft Materials Research Center*
*Department of Physics, University of Colorado.*

*https://smrc.colorado.edu*