



## ~~~~ Polymer Physics Seminar ~~~~

### Huai Suen Shiau

Chemical Engineering, Penn State University

Advisor: Professor Michael J. Janik and Ralph H. Colby

10:00 AM Tuesday September 6<sup>th</sup>, 2011  
301 Steidle Bldg.

### Computationally aided design of ionic polymer electrolytes for facile ion transport

Ion-containing polymers have drawn much attention because they offer significant advantages as polymer electrolytes in Li-ion batteries. However, current ion conductivities are too small for practical applications, suggesting further optimization towards promoting dissociation of the anion-cation interaction could enhance conductivity. An quantum-chemical investigation on the Li-anion poly(ethylene oxide) system was performed by developing cluster-continuum model (CCM) to approximate the solvating effects of the polyethylene oxide on the anion-cation structures, from which we estimated the relative concentration of various Li ion states, and estimate the energy barriers to Li<sup>+</sup> hopping between ion pairs. The result showed that more diffuse anions increase the fraction of mobile Li<sup>+</sup> ions by weakening the anion-cation interaction and predicted concentrations are compared among a series of anions to indicate favorable features for selection of an optimal Li<sup>+</sup> ionomer. In order to design Li-anion system with high ion mobility, we explored Li<sup>+</sup> conduction mechanism via hopping among various states using *ab initio* method. At small anion separations, the Li<sup>+</sup> hopping barrier is low and solvent-separated triple ions are more stable than contact triple ions. Future work will be to develop an integrated *ab initio*-kinetic Monte Carlo (kMC) model in order to investigate the dynamic evolution of Li<sup>+</sup> hopping among various states in ionomers.