



## ~~Special Polymer Physics Seminar ~~

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**10:00 AM Tuesday, June 22<sup>th</sup>, 2010**  
**301 Steidle Bldg.**

### **Developing Coarse-Grained Models for the Molecular Simulation of the Self Assembly of Skin Lipids**

The outermost layer of the skin (the stratum corneum) consists of skin cells embedded in a rich lipid matrix, whose primary role is to provide a barrier to foreign agents entering the body and to water leaving the body. This lipid system is unique in biological membranes in that it is composed of ceramides, cholesterol, and free fatty acids, with phospholipids, which are the major components of most biological membranes, being completely absent. This unique composition enables the organization of the stratum corneum lipids into lamella, which in turn is believed to control the barrier function of the skin. While much is known about the nature of the skin lipids from extensive experimental studies, a clear understanding of how and why these molecules assemble into the structures observed through microscopy and biophysical measurements does not yet exist. In order to probe the molecular level arrangement, we have developed coarse-grained models for key stratum corneum lipids and water to enable us to simulate complex mixed lipid systems and study their structural characteristics on timescales accessible to molecular dynamics simulations. Results of simulations performed in the development of the coarse-grained models will be presented alongside the results of self-assembly studies that enable us to validate the models developed.