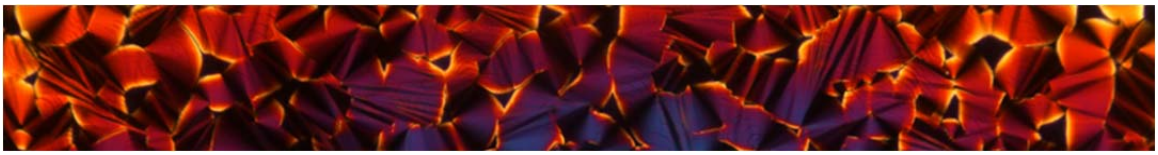

LIQUID CRYSTAL MATERIALS RESEARCH CENTER

SPECIAL SEMINAR SERIES

Molecular Simulations of the Melting and Mechanical Properties of Polymer Grafted Bilayer Membranes

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Understanding the influence of grafted polymers on the physico-mechanical properties of bilayer membranes is important in drug delivery and cosmetics. In this talk I will present an overview of our work concerning the phase behavior of surfactant membranes using both atomistic and coarse grained molecular dynamics simulations. Using all atom molecular dynamics simulations, the melting characteristics of surfactant membranes as a function of co-surfactant concentration illustrates the rich variety of phase behavior in the behenyl trimethyl ammonium chloride (BTMAC) – stearyl alcohol- water, lamellar phase. In a certain range of stearyl alcohol concentration, the ripple phase with 1 and 2D symmetry is observed in the gel phase. The changes in the bilayer microstructure and bending moduli of polymer grafted bilayers are investigated using dissipative particle dynamics simulations as a function of the amount of grafted polymer and surfactant chain length. For shorter chain molecules the transition from the low temperature gel phase to the liquid crystalline phase is lowered only above a grafting fraction of 0.12. Below a grafting fraction of 0.12 small changes are observed only for the thinner bilayers. The bending modulus of the bilayers is obtained as a function of the grafting fraction. Using a mean field theory developed for polymer grafted membranes, the contributions to the changes in the bending modulus from bilayer thinning were found to lie within 11% the shorter chain molecules, increasing to 15% for the longer chain molecules. The increase in the area per head group of the lipids was found to be consistent with the scalings predicted by self-consistent mean field results.

Friday, April 12th at 1:30 p.m. Duane Physics G1B31

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