Dear Faculty, IGERT Fellows, IGERT Associates and Students,

You are cordially invited to attend a Seminar presented by Jillian Larsen. Please plan to attend.

Jillian Larsen

IGERT Fellow

Date: Friday, March 7, 2014 Location: Bourns A265 Time: 11:00am

Dipole modulated charge transfer and tools for experimental molecular mechanics

Abstract:

Controlling charge transfer at the nanometer scale is a critical component for efficient light harvesting and energy conversion. Since local electric fields provide a means for "steering" electron transduction, the use of molecular electrets presents an important paradigm for energy engineering. An "electret," or specifically, a "dipole-polarization electret," is an electrostatic analogue of a magnet. An electret contains co-directionally ordered permanent electric dipoles. Protein alpha-helices are the best example of molecular electrets, with intrinsic dipoles of 5 Debyes per residue, which generate nanometer-scale electric fields of Gigavolts per meter. The ordered hydrogen-bonding network and amide linkages are responsible for the intrinsic dipole moments of protein alpha-helices. Although the intrinsic dipoles of these biopolymers can rectify electron transfer and aid ion transport, the direct use of protein helices as electronic materials is challenging because of their large band gaps, inability to efficiently mediate electron transfer beyond 2 nm, and conformational sensitivity. Therefore, we have undertaken a bioinspired approach in the design of molecular electrets that possess all advantages that protein helices have to offer (i.e., ordered amide and hydrogen bonds that generate intrinsic dipoles of about 4 Debyes per residue). Unlike their biological macromolecular counterparts, the bioinspired electrets can mediate efficient long-range charge transfer along their backbones. An in-depth structure-function analysis of the electret systems, however, revealed that molecular motions causing conformational changes had a dominating effect on the way dipoles modulate the charge-recombination kinetics. Indeed, conformational gating and molecular dynamics can drastically affect the kinetics of charge-transfer processes, thus, having important implications for the efficiencies of photovoltaics and other energy-conversion and storage technologies. To gain further understanding of these important structural features, we are developing a magnetoptical system for experimental probing of molecular dynamics at a single-molecule level. In Magnetic tweezers, or more specifically, Magnetic pullers systems, tested molecules are attached to the surface of a microscope slide and to magnetic microspheres. The magnetic microspheres have dual role: they are force transducers and optical probes for the molecular motions. X-Y movement of the microspheres along the focal plane provides a means for follow the lateral motion of microscopic object. By incorporated Reflectance Interference Contrast Microscopy (RICM) in our magnetic pullers the vertical component of these motions, i.e., the Z-component of the movements normal to the focal plane, can be measured. Our ability to measure charge-transfer kinetics with femtosecond resolution will complement the molecular dynamics that the RICM video recordings can provide. This synergy will allow us to gain understanding of the structure-function relationship between dipole-modulated

charge transfer and molecular dynamics. In particular, we will elucidate how the presence of local electric fields, combined with controlled conformational gating, can improve energy-conversion efficiencies.

