

# Physical Chemistry Seminar



**Professor**

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## *The Relation Between Structural and Electronic Order in Organic Photovoltaic Materials*

It is well known that conjugated polymers are difficult to study because the optical and electronic properties of the polymer are highly dependent on the processing history, and thereby the structural order. We report on the fabrication and characterization of crystalline nanofibers of regio-regular poly-3-hexylthiophene (rr-P3HT). Nanofibers that are formed slowly display highly aligned domains of crystalline polymer and display absorption and emission spectra that are consistent with a J-aggregate. By comparison, nanofibers that are formed quickly display smaller and less well aligned crystalline domains and display absorption and emission spectra consistent with an H-aggregate. We detail spectroscopy that verifies our assignments and analysis of the how control of fabrication steps leads to increased structural order. This culminates in predictive molecular dynamics modeling of polymer nanoparticle formation in solution.

These molecular processes of domain formation, phase separation, and crystallization occur every time a bulk-heterojunction organic photovoltaic (BHJ-OPV) film is formed. The fibers we isolate for spectroscopy exist in complete devices. For the second half of the talk I will detail electron microscopy and neutron scattering techniques that we used to determine the nano and microscopic morphology of the materials. It is the hierarchical nature of the morphology that ultimately allows BHJ-OPV layers to function. I will show how the different length scales fit together.

**Monday, October 14, 2013**

**4:00 P.M.**

**2033 Young Hall**