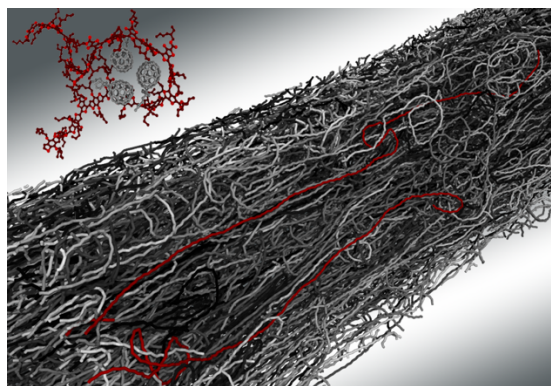


Samuel Evan Root Dissertation Defense
Chemical Engineering Ph.D. Candidate
The Lipomi Research Group
Tuesday, February 13, 2018
2:00p.m.
Funq Auditorium

“Mechanical Properties of Polymeric Semiconductors: From Molecular Simulations to Process Design”

PI: Dr. Darren Lipomi

Abstract: Softness and mechanical deformability underpin most of the advantages offered by polymeric semiconductors. A detailed understanding of the mechanical properties of these materials is crucial for the design and manufacturing of robust, thin-film devices such as solar cells, displays, and sensors. The mechanical behavior of polymers is a complex function of many interrelated factors that span multiple scales, ranging from molecular structure, to microstructural morphology, and device geometry. This thesis builds a comprehensive understanding of the thermomechanical properties of polymeric semiconductors through the development and experimental-validation of computational methods for mechanical simulation. A predictive computational methodology is designed and encapsulated into open-sourced software for automating molecular simulations on modern supercomputing hardware. These simulations are used to explore the role of molecular structure/weight and processing conditions on solid-state morphology and thermomechanical behavior. Experimental characterization is employed to test these predictions—including the development of simple, new techniques for rigorously characterizing thin-film thermo-mechanics. Knowledge acquired from this fundamental research is employed to design a continuous manufacturing process: **interfacial drawing**, which leverages the spontaneous spreading and drying of a polymer solution at the surface of water to fabricate high-quality thin films over large areas.



Biosketch: Samuel E. Root is from Great Neck, New York. He completed his B.S. in chemical engineering with a minor in applied mathematics at University of Rochester, 2014.