



Polymers under Multiple Constraints

# Polymer- & Soft-Matter-Seminar

**Prof. Dr. Jutta Luettmmer-Strathmann**

(Prof. Dr. Jutta Luettmmer-Strathmann, University of Akron, Ohio, USA)

**TUESDAY,  
4<sup>th</sup> July 2017**

**at: 5.15pm**

**VDP4 1.27,  
Von-Danckelmann-Platz 4,  
06120 Halle**

## **“INVESTIGATIONS OF SEXITHIOPHENE PROPERTIES WITH MONTE CARLO SIMULATIONS OF A COARSE-GRAINED MODEL”**

Thiophenes have important applications in organic electronics, energy conversion, and storage. In this study, we focus on  $\alpha$ -sexithiophene ( $\alpha$ -6T), a small,  $\pi$ -conjugated molecule whose visible light absorption and high charge carrier mobility make it interesting for applications. While the structural properties of  $\alpha$ -6T have important effects on device performance, the structure of  $\alpha$ -6T is not easy to model. In this work, we develop a coarse-grained model for alpha-oligothiophenes in the bulk. Since a-sexithiophene is a six-ring molecule, we describe it as a linear chain of bonded, discotic particles with Gay-Berne potential interactions between non-bonded ellipsoids. We perform Monte Carlo simulations of our coarse-grained model to investigate single-molecule, structural, and thermodynamic properties of  $\alpha$ -6T over a large range of temperatures. Our results show a crystalline state with herringbone structure at low temperature, an isotropic liquid at high temperatures, and liquid crystalline phases in between. This is in qualitative agreement with experimental and atomistic simulation data from the literature.