



Polymers under multiple constraints:
restricted and controlled molecular
order and mobility

Polymer- & Soft-Matter- Seminar

Tuesday,
3rd July 2012

at: 5.15 pm

VDP 1.27
Seminarraum
Chemie,
Von-Danckel-
mann-Platz 4,
06120 Halle

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“Assessing Packing Organization and Local Molecular Dynamics in Func- tional Organic Materials”

Functional organic materials with extended π -conjugation, such as low band gap polymers and disc-shaped molecules, are important technological materials with the potential to serve as efficient organic semiconductors in various electronic devices. A common feature shared by most of these materials is that their specific function is established via solution processing. This process utilizes the spontaneous self assembly of molecules driven by entropy and it results in materials with regions of high and low order, often referred to as semi crystallinity. The absence of long range ordering, however, prevents the direct access to details about the local molecular organization from a conventional approach.

In my talk I will outline a general strategy for determining the packing organization in semi-crystalline polymers that takes advantage of several experimental methods (X-ray diffraction, solid-state NMR, and other techniques) in combination with quantum chemical calculations. This provides a useful platform to assess specific packing motifs and in some cases even allows setting up a crystal structure, if constraints about the packing organization can be derived from experiments. The potential of the proposed strategy will be exemplified by recent and ongoing work on low band gap polymers, P3HT and donor-acceptor-type polymers [1,2], and shape-persistent macrocycles, forming empty helical nano channels [3]. Finally, I will illustrate how site-specific information about molecular dynamics from solid-state NMR experiments can be used to elucidate complex motions in discotic liquid crystals [4-7].

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