

Segmental mobility in polymer melts, polymer blends and polymer electrolytes

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This talk focuses on the investigation of the segmental mobility in various polymeric systems by means of MD simulations. In the first part, a novel statistical method will be introduced, which allows one to characterize the Rouse mobility of individual polymer segments. Since this approach is based on the local Langevin equation, it complements the classical, nonlocal Rouse mode analysis, and is thus ideally suited to quantify the segmental motion in systems for which the Rouse assumption breaks down. As an example, I will discuss a dynamically heterogeneous PEO/PMMA blend. The second part is dedicated to the polymer mobility in ternary polymer electrolyte-ionic liquid mixtures, which are promising ion conductors for lithium ion batteries. Here, special emphasis is put on the importance of the segmental motion for the macroscopic lithium ion transport.

Friday, 22nd March
10:00 am
Seminarrom 1.079
Allmandring 3