Polymers under Multiple Constraints

Polymer- & Soft-Matter-Seminar

Tuesday,
2nd May 2017

at: **5.15pm**

VDP4 1.27,
Von-Danckel-mann-Platz 4,
06120 Halle

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“The Balance of Interactions in Ionic Liquids"

As a newly emerging class of solvents with many promising properties, ionic liquids have received considerable attention during the last decade. These compounds can exhibit a certain degree of long-range ordering, or even microphase separation, despite of being liquids, which typically possess only local order. This complex behavior is a consequence of the subtle balance of different kinds of interactions. In this contribution, the method of molecular dynamics (MD) simulation is presented as a powerful tool to investigate these phenomena. Many relevant properties which are typically determined in experiments - such as structure factors from X-ray scattering, or IR/Raman spectra - can be directly obtained from MD simulations, making it able to compare those to the experimental results. This can help to assign specific features in the experimental data to the underlying microscopic processes, and therefore to gain a better understanding of this class of substances.

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IOM Leibniz Institute of Surface Modification

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