Martin-Luther-Universität Halle-Wittenberg
Naturwissenschaftliche Fakultät II
Chemie und Physik
SFB TR 102

POLYMER- UND SOFT-MATTER-KOLLOQUIUM

am Dienstag, dem 22.11.2011, 17.15 Uhr,

„Gustav Mie“ Hörsaal E.08, Theodor – Lieser - Str. 9, 06120 Halle

Es spricht:

Frau Dr. H.-P. Hsu
Institut für Physik,
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zum Thema:

"Conformational properties of stretched and unstretched semiflexible polymer chains”

Abstract:

Semiflexible polymer chains under good solvent conditions are described by self-avoiding walks on the square and simple cubic lattices in d=2 and d=3 dimensions, respectively, and the stiffness of chains is controlled by the bending energy. With the pruned-enriched Rosenbluth methed (PERM), we observe a double crossover behavior, rigid-rod-like to (almost) Gaussian random coils, then to self-avoiding walks, for the chain length up to N=50000 in d=3, but only a single crossover from rigid-rod-like to self-avoiding walks for the chain length up to N=25600. in d=2.
Testing the applicability of the Kratky-Porod model, we also check whether the chain conformation is dominated by the excluded volume effects or not as the chain length and its flexibility vary.
However, the extension versus force curve is still not well understood if the stretching force is applied to one end of polymer chains although a plenty of literature exits. We therefore extend our study to the problem of stretching semiflexible chains.
Varying the strength of the force, the flexibility of the chain, and the chain length, the theoretical predictions of the force-extension relationship at different length scale regimes (linear response - Pincus blob - Kratky-Porod model - freely joined chain) are checked. Our large scale Monte Carlo simulations give clear evidence for the importance of excluded volume effects on the stretching behavior of semiflexible polymer chains.