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

Polymer Physik-Seminar

am Dienstag, dem 22.05.2012, 14.15 Uhr

SR 102, VSP1, Von-Seckendorff-Platz 1,
06120 Halle

Es spricht: **Dr. Vakhtang Rostiashvili,**
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Mainz

Titel :

"Driven and undriven translocation of a polymer chain: between dynamical scaling and molecular dynamic simulation"

Abstract:

Translocation dynamics is an essential component of transport in biological cells. Most of the experimental studies deal with a driven polymer translocations that is realized by applying an electrical field across a narrow pore. We suggest a theoretical description of the force-induced translocation dynamics of a polymer chain through a nanopore. Consideration is based on the tensile blob picture of a driven chain and the notion of a propagating front of tensile force along the chain backbone, suggested by Sakaue (Phys. Rev. E 81, 041808 (2010)).
The driving force is associated with a chemical potential gradient that acts on each chain segment inside the pore. Depending on its strength, different regimes of polymer motion (named after the typical chain conformation, ``trumpet'', ``stem-trumpet'', ``stem'') occur. Assuming that the local driving and drag forces are equal (i.e., in a quasi-static approximation), we derive an equation of motion for the tensile front position. We show that the scaling law for the average translocation time versus chain length changes as the driving force f grows. As a result the corresponding scaling exponent increases with f.
This and other predictions are tested by Molecular Dynamics (MD) simulation. Data from our computer experiment indicate indeed that the translocation scaling exponent increases with the pulling force f albeit the observed exponent stays systematically smaller than the theoretically predicted value. In order to study the role of fluctuations (which are ignored in the quasi-static approximation), we suggest a governing Fokker-Planck Equation for the translocation coordinate probability distribution function W(s,t). It is shown that at least for the undriven translocation the process could be rationalized within the framework of fractional Brownian motion (fBm). In particular, this means that W(s,t) is Gaussian but with a time-dependent variance which grows subdiffusively. These results are supported by extensive MD-simulation performed in 3D.