



"Soft-Matter Seminar"

Felix Hanke

Department of Physics and Atmospheric Science Dalhousie University
Halifax, NS B3H 3J5 Canada

The mechanical response of single polymers in and out of equilibrium

During this talk, several aspects of the theory of single molecule stretching are discussed. The Transfer Matrix method is used throughout, hence the talk will start with a short primer. Next, a statistical theory is presented which is aimed at understanding conformational transitions, a feature commonly observed in single molecule stretching experiments. This so-called continuous two-state model is initially developed in the Gibbs ensemble where it can be used directly to fit force-extension data. These fitting results are then substituted into an independent Transfer Matrix calculation to reproduce the observed thermal fluctuations in the Helmholtz ensemble. The possibility and magnitude of temperature dependences in conformational transitions is also demonstrated.

The second half of the presentation will deal with a theory for fast polymer stretching, which would be necessary to model AFM experiments at high pulling speeds and loading rates. Using exact Transfer-Matrix based equilibrium statistical mechanics and the simplest possible transition rates in a Master Equation formalism, it is possible to predict the mechanical response of molecules that are stretched on time scales faster than their relaxation time. Finally, single molecule relaxation within this Master equation frame work will be discussed.

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Sonderforschungsbereich 563, Bioorganic functional systems on solids
Prof. Dr. Roland Netz
Physik-Department T 37, Technische Universität München, Theoretische Physik
85747 Garching