Polymers under Multiple Constraints

Polymer- & Soft-Matter-Seminar

Tuesday,
10th December
2013

at: **2.15** pm

VSP1 SR 1.02,
Von-Seckendorff-Platz 1,
06120 Halle

Special Event

Prof. Mark P. Taylor

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"Adsorption and folding transitions of a polymer chain: Applications of the Wang-Landau and partition function zeros methods"

The Wang-Landau (WL) algorithm is a Monte Carlo simulation technique providing a direct computation of the density of states (and thus the partition function) of a many-body system. The partition function encodes all thermodynamic information about a system, and thus, its construction allows for an efficient determination of phase behavior. Here we describe the application of the WL approach to continuum interaction-site polymer chains and compute single-chain phase diagrams for both flexible and semi-flexible homopolymer chains and for a flexible AB-heteropolymer chain [1]. Distinctive folded chain morphologies are observed for the semi-flexible and heteropolymer chains. We also use the WL approach to study the adsorption transition of a flexible lattice chain tethered to an attractive surface. In this latter case we analyze the zeros of the canonical partition function in the complex inverse-temperature plane [2]. These zeros define a nearly closed circular region, centered on the origin, intersected near the positive real axis by two flaring tails. With increasing chain length the intersection point pinches down towards the positive real axis, dividing the real axis into two distinct regions or phases in accord with Yang-Lee theory. We apply finite size scaling theory for the leading partition function zeros to locate the adsorption transition in the thermodynamic limit and obtain values for the polymer crossover, order parameter, and specific heat exponents.

[1] M.P. Taylor, W. Paul, and K. Binder, Polymer Science, Series C 55, 23 (2013).
[2] M.P. Taylor, P.P. Aung, and W. Paul, Phys. Rev. E 88, 012604 (2013).