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

POLYMER- UND SOFT-MATTER-KOLLOQUIUM

am Dienstag, dem 29.11.2011, 17.15 Uhr,

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

Es spricht:

Prof. Dr. M. P. Taylor
Department of Physics,
Hiram College, USA

zum Thema:

“Partition function zeros, configuration landscapes, and phase transitions of a polymer chain”

Abstract:

A single polymer chain can undergo a series of conformational transitions analogous to the phase transitions exhibited by bulk materials. We have recently studied the conformational transitions of a flexible square-well polymer chain using a Wang-Landau simulation approach in which we directly compute the single-chain partition function. The temperature-interaction range phase diagram for this homopolymer includes both a coil-globule and globule-crystal transition as well as an "all-or-none" coil-crystal transition [1]. Here we study these conformational transitions in more detail by analyzing the zeros of the single-chain partition function and by constructing a 2D configurational probability landscape. Each of the above single-chain transitions is found to display a well-defined signature in the complex-plane map of the partition function zeros. The freezing transition is characterized by a nearly circular ring of uniformly spaced roots while the collapse transition is signaled by the coalescence of roots onto an elliptical horse-shoe segment pinching down towards the positive real axis. For sufficiently small interaction range, the elliptical collapse ring merges with the circular freezing ring yielding the direct coil-crystal transition. The root density of these rings increases with increasing chain length and the leading roots move towards the positive real axis, implying a divergence of the specific heat in the thermodynamic limit (as originally proposed by Yang and Lee). The 2D configurational landscape reveals a dominant "folding" pathway that includes an inherent configurational barrier or bottleneck to single-chain freezing associated with the formation of a transition state structure (i.e., crystal nucleation).

[1] M.P. Taylor, W. Paul, and K. Binder, J. Chem. Phys. 131, 114907 (2009).