Polymers under Multiple Constraints

Polymer- & Soft-Matter-Seminar

Prof. Mark P. Taylor

(Departments of Physics, Hiram College, USA)

Tuesday,
30th April 2019

at: **5.15pm**

VDP 4 1.27,
Von-Danckelmann-Platz 4
06120 Halle

"Folding of a model biopolymer in a crowded environment"

At the molecular level, biological systems operate in very crowded solution environments. It has long been recognized that this crowding can affect the conformational stability and phase transitions of the biopolymers comprising such systems. Similar issues must be addressed in developing biotechnology applications based of dense arrays of surface-tethered polymers. In the case of macromolecular folding it is generally assumed that crowding (and geometric confinement) will favor the folded state due to excluded volume effects drastically reducing the number of accessible unfolded states. In our recent work we directly measure this type of crowding/confinement induced entropy reduction using Wang-Landau computer simulation techniques.

In this talk we will first discuss some general results on crowding and confinement for a simple polymer system [1] and will then address the folding transition of a specific single-stranded DNA oligomer that has been studied extensively by the group of Plaxco [2]. We develop a coarse-grained model for this ssDNA and use it to examine the entropic effects associated with both surface tethering and surface crowding. Contrary to the simple entropic considerations noted above, we find that tethering (a form of confinement) slightly destabilizes the folded state. For the tethered ssDNA oligomer crowded by other tethered oligomers, we find, in agreement with experiment, that both stabilization and destabilization are possible depending on the conformational state of the crowders.

[1] Taylor, Macromolecules 50, 6967 (2017); J. Chem. Phys. 147, 166101 (2017).
[2] Watkins et al, JACS 134, 2120 (2012); JACS 136, 8923 (2014).