Theoretical Polymer Physics

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"Polymer folding in confined and crowded environments "

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VSP 1 1.26, Von-Secken-dorff- Platz 1, 06120 Halle

A flexible homopolymer chain with sufficiently short-range inter-actions undergoes a first-order-like transition from an expanded coil to a compact crystallite. We have recently shown that this very simple model illustrates the underlying polymer physics leading to the distinct all-or-none folding thermodynamics characterizing many small proteins [1]. Here we investigate this polymer folding transition under geometric confinement and in the presence of macromolecular crowders. One anticipates that both confinement and crowding will reduce the entropy of the unfolded chain, thereby stabilizing the folded state and shifting the transition to higher temperature. We use a Wang-Landau simulation approach to construct the partition function of a flexible square-well-sphere chain (monomer diameter d) that is (A) confined within a hard-wall slit or cylindrical pore and (B) immersed in a hard-sphere solvent with solvent diameter $D \geq d$ and solvent volume fraction $0 < vf \leq 0.4$. Entropic stabilization of the folded state is found in all cases. For the confined chain, isothermal reduction of the slit width or cylinder diameter can induce folding, unfolding, or crystallite restructuring. In the crowded environment an isothermal increase in the crowder density can induce folding. This crowding behavior is sensitive to the size of the crowder with larger crowders producing a smaller effect. Both phase diagrams and quantitative analyses of entropy reduction and changes to the free energy barrier to folding will be presented.

[1] Taylor, Paul, and Binder, J. Chem. Phys. 145, 174903 (2016)

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