Interdisciplinary Master’s research project at Eindhoven University of Technology

Title: Statistical thermodynamics of the folding of single-chain polymer nanoparticles

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Abstract: Grafting supramolecular motifs onto a polymer backbone is a versatile route towards foldable polymers. We use a special class of such motifs, namely benzene-1,3,5-tricarboxamides (BTAs) to ‘fold’ water-soluble polymers into ‘single-chain polymer nanoparticles’ (SCNPs) that can be used as water-borne sensors and catalysts. A graphical representation of a SCNP is given below. Recent small-angle scattering experiments on SCNPs in water/alcohol mixtures demonstrated for the first time that directional interactions between the grafted BTAs can indeed dramatically alter the polymer conformation. In this final year Master’s research project at the interface between chemistry and physics you will develop a theoretical model in order to better understand the relation between the conformation of the polymer and its chemical composition, molar mass, and the spontaneous assembly of pendant BTAs. An important aspect will be elucidating how the conformational frustration of the polymer backbone interferes with the tendency of the BTAs to form supramolecular stacks in solution. An interest in polymers, self-assembly, statistical thermodynamics and modelling is a prerequisite. Experience in using the Mathematica and/or Mathlab computer packages is not required but would be advantageous.