NEUTRAL AND CHARGED DENDRON BRUSHES: STRUCTURE AND PROPERTIES

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Polymer brushes - monolayers of polymer chains densely grafted onto impenetrable substrates - belong to the most popular and intensively studied polymer systems. In the last few years there exists a huge interest to a new class of polymer brushes, where not the traditional linear chains but macromolecules of branched topologies, in particular, regularly branched dendrons, are grafted onto a substrate. Theoretical and simulation approaches typically used to study dendron brushes include Monte Carlo and molecular dynamic simulation, self-consistent field numerical methods, and various analytical approaches.

Theoretical studies revealed that dendron and star brushes (the star brush is equivalent to the first generation dendron brush) have specific properties that are associated with their non-trivial internal structure. At high grafting densities, dendrons' packing in a planar brush results in a relatively uniform and smooth density profile. Because of the branched architecture of grafted macromolecules, this can be achieved by separation of dendrons into two or more groups, or populations, differing in the degree of stretching. This remarkable feature of dendron brushes will be discussed in detail. Effect of the charge on the structure of dendron brushes will be discussed, both cases of polyelectrolyte dendron brushes with fixed charge and pH-sensitive dendron brushes will be considered.

The peculiarities of the internal structure of dendron brushes allows using them as matrices for "molecular switches". To demonstrate this, the behavior of a single linear chain embedded into a star brush well be considered. It will be shown that the chain may undergo sharp conformational coil-to-flower transition triggered by a change in the brush grafting density or in the solvent quality (equivalent to temperature variation). Thus, it is possible to control the linear chain conformation by changing the properties of the matrix. In the case of dendron polyelectrolyte brushes, the number of ways to control the brush properties increases (one can vary the ionic strength or the degree of ionization), and in the final part of the talk the behaviour of a non-charged chain in a polyelectrolyte star brush will be discussed.

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