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Surface-induced alignment of liquid crystalline dendrimers

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Dendrimers are a class of monodisperse polymeric macromolecules with a well-defined and highly branched three-dimensional architecture. Liquid crystalline dendrimers (LCDrs) are usually derived through functionalization of common dendrimers with low molar mass liquid crystal molecules (mesogens) [1, 2]. The ability to control the macroscopic alignment of LCDrs is a key factor for many of their potential applications. For low molar mass liquid crystals (LC), robust and well-established techniques/materials are available for the precise alignment of the LC medium through surface-mediated interactions. Through controlling the surface-LC interactions, usually by means of chemical and/or mechanical treatment of the substrate, a variety of alignments (homeotropic, planar, tilted, etc.) of the LC medium with respect to the substrate are possible. The situation in LCDrs is quite different due to the rather strong positional/orientational constrains between the interconnected mesogenic units of the same dendrimer. Therefore the surface-mediated alignment in the case of LCDrs is determined by the fine interplay between the anchoring driven alignment of the mesogenic units and by the constraints the dendritic architecture imposes on them. We introduce a tractable coarse-grained force field for the inter-dendritic and the dendrimer-substrate interactions [3]. Based on this we present results from Monte Carlo simulations of LCDrs i) adsorbed on flat, impenetrable aligning substrates and ii) confined into nanopores of different geometries. Depending on the anchoring constrains to the mesogenic units of the LCDr and on temperature, a variety of stable ordered LCDr states, differing in their topology, are observed and analysed. The influence of the dendritic generation and core functionality on the surface-induced ordering of the LCDrs are examined.

References

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