

Molecular Simulation Study of Confined Liquid Crystalline Systems

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Liquid crystals (LC) are states of matter that exhibit thermodynamic, kinetic, and structural properties between those of isotropic liquids and crystalline solids. These mesophases simultaneously possess liquid-like properties, such as an ability to flow, and crystal-like properties, including long-range orientational order and anisotropic optical features. For many LC-based technologies mesogens are restricted to highly confined environments or are otherwise brought into intimate contact with a surface. In such cases the behavior exhibited by the fluid can be very different from that observed in the bulk. In this work we use molecular simulation to probe the phase behavior of bulk and nanoconfined LC systems. Specifically, we use transition-matrix Monte Carlo simulation to examine the behavior of the hard Gaussian overlap model confined between parallel plates. Mesogens interact with the substrate via a hard needle wall potential, which controls the extent to which molecules can penetrate the surface. Our results point to a sequence of interesting transitions with variation of the needle length. Wetting transitions are observed with short (long) needles wherein the nematic director oriented perpendicular (parallel) to the wall wets the substrate. Anchoring transitions are also found at intermediate values of the needle length.