Surface Ordering and Capillary Phenomena of Confined Hard Cut-Sphere Particles

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The effects induced by a solid surface on liquid crystal phases have attracted great interest over the last decades due to the wide variety of phenomena arising at the interface, and their promising technological applications. The presence of a solid surface causes a breaking in the symmetry of the system that alters the structure of the liquid crystal phase, and modifies both its thermophysical properties and its phase diagram. These effects, although related, may be classified into three different categories: surface ordering, anchoring and wetting. In this work, the confinement of a discotic liquid crystal composed of hard cut spheres of aspect ratio L/D=0.1 in a slit pore formed by two parallel hard walls has been studied, including the capillary process induced by the width variation in the slab geometry. The study is focused on the isotropic nematic transition region, which has been characterized using Monte Carlo molecular simulations in the isothermal-isobaric (NPT) and Gibbs ensembles. Two different types of confining walls were considered, the first of them being completely hard, i. e., excluding the whole mesogen volume, and the other one partially adsorbent, excluding only the centre of mass of the cut sphere. The difference between the influences of each type of wall on the liquid crystal bulk has been analysed. First, the order induced nearby the surfaces by the confinement has been characterized through the density and order parameter profiles. Then, the displacement of the isotropic nematic transition, which is dependent on the pore size, has been determined, leading in each case to different nematization or isotropization capillary phenomena.