Liquid-crystal patterns of rectangular particles in a square nanocavity

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Using density-functional theory in the restricted-orientation approximation, we analyse[1] the liquid-crystal patterns and phase behaviour of a fluid of hard rectangular particles confined in a two-dimensional square nanocavity of side length H composed of hard inner walls. Patterning in the cavity is governed by surface-induced order, capillary and frustration effects, and depends on the relative values of particle aspect ratio $\kappa \equiv L/\sigma$, with L the length and σ the width of the rectangles ($L \geq \sigma$), and cavity size H. Ordering may be very different from bulk ($H \to \infty$) behaviour when H is a few times the particle length L (nanocavity). Bulk and confinement properties are obtained for the cases $\kappa = 1$, 3 and 6. In bulk the isotropic phase is always stable at low packing fractions $\eta = L\sigma\rho_0$ (with ρ_0 the average density), and nematic, smectic, columnar and crystal phases can be stabilised at higher η depending on κ: for increasing η the sequence isotropic $\to$ columnar is obtained for $\kappa = 1$ and 3, whereas for $\kappa = 6$ we obtain isotropic $\to$ nematic $\to$ smectic (the crystal being unstable in all three cases for the density range explored). In the confined fluid surface-induced frustration leads to four-fold symmetry breaking in all phases (which become two-fold symmetric). Since no director distorsion can arise in our model by construction, frustration in the director orientation is relaxed by the creation of domain walls (where the director changes by 90°); this configuration is necessary to stabilise periodic phases. For $\kappa = 1$ the crystal becomes stable with commensuration transitions taking place as H is varied. These transitions involve structures with different number of peaks in the local density. In the case $\kappa = 3$ the commensuration transitions involve columnar phases with different number of columns. Finally, in the case $\kappa = 6$, the high-density region of the phase diagram is dominated by commensuration transitions between smectic structures; at lower densities there is a symmetry-breaking isotropic $\to$ nematic transition exhibiting non-monotonic behaviour with cavity size. Apart from the present application in a confinement setup, our model could be used to explore the bulk region near close packing in order to elucidate the possible existence of disordered phases at close packing.

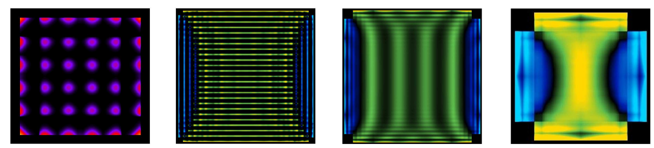

FIG. 1. Equilibrium density profiles for different conditions of rod aspect ratio, chemical potential and cavity size. From left to right they are shown crystal, columnar, smectic and nematic phases respectively. Yellow/green colors represent particles with their director paralell to x-axis and blue color means particles paralell to y-axis. The crystal phase is different because it comes from a system with aspect ratio 1 (squares) so color only represents density value.

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