Chapter 7

Conclusions

Computer simulation methods are proving to be efficient tools to study complex molecular structures in interesting soft materials like confined liquid crystals under chosen boundary conditions. This thesis reports results of such investigations in a variety of such systems. A hybrid film of uniaxial molecules was studied using non - Boltzmann sampling methods. Thin films confined between substrates inducing competing boundary conditions were studied by varying the temperature, the anchoring strength of the substrates and the thickness of the liquid crystal film. These novel sampling methods provided relatively free estimates of different parameter as a function of finely controlled temperature. This study helped in characterizing this transition more reliably and accordingly, providing more readily observable physical variables to detect the onset of new phases. As a special case to hybrid films, a thin film of liquid crystals was confined between two cylindrical substrates inducing order in perpendicular directions. Due to the curvature present in the system the elastic energy (different at the two substrates due to differing curvatures) plays an important role. A biaxial phase in this system is observed when the anchoring strength of the two substrates is carefully tuned to induce balanced competing influences on the intermediate layers of the system. The biaxial phase observed in these hybrid films is due to the confinement effects on uniaxial liquid crystal molecules, and in classified as phase biaxiality.

In reality liquid crystal molecules are known to have finite molecular biaxiality. For simplicity, they are mostly modeled as uniaxial rod - like or disc - like molecules. Curiosity lies in understanding as to why a macroscopic biaxial order is not observed when

the liquid crystal molecules are themselves are microscopically not symmetric around their long axes. From the point of experiments, unambiguous acceptance of the realization of a biaxial phase is counting to be a challenging question to be resolved. In this context predictions based more general Hamiltonian models could be useful in understanding the molecular origin for observation of macroscopic biaxial symmetry. Accordingly, molecular modeling of a biaxial liquid crystal was attempted in order to lead to the possibility of determining microscopic criteria for realistic biaxial liquid crystal. A general model incorporating two parameters was used for this study (equation 1.5.4). Phase diagrams were computed with the variation of the two parameters (Γ, Λ). These predictions are new, and are interesting from the point of view of developing appropriate criteria at a molecular level for the observation of a biaxial phase.

Such studies on biaxial liquid crystals were extended was studied hybrid films, realized by applying competing boundary conditions creating restrictive constraints. It was observed that for such confined systems there are two biaxial phases possible at low temperature. The phase formed immediately below the isotropic phase is a biaxial phase exclusively due to the phase biaxiality, arising from the self - organization of the long axes of the molecules. The lower temperature biaxial phase is primarily due to the molecular biaxiality arising from the interacting biaxial components of the molecules. This system was further studied by varying the relative anchoring strengths of the substrates keeping. It is seen that there exists a threshold anchoring strength beyond which there is an abrupt change in the director structure, and consequently the associated physical parameters.

Finally a liquid crystal droplet confined in a polymer is revisited using canonical Monte Carlo studies. The Hamiltonian used for this study has the facility to include elastic constants as parameters that can be varied independently. The droplet considered has been subjected to radial anchoring at the polymer surface, so that one need to consider only splay distortion as the relevant condition in the Hamiltonian. With the variation in the anchoring strength sudden transition between two qualitatively different structures is observed. This system is further by varying the splay elastic constant and on finds that it affects both the

threshold anchoring strengths, as well as the size of the inner uniaxial core. The reliability of the computations and the applicability of the model were investigated by changing the spatial extent over which the director is defined. The anchoring transition reported in this study exhibits strong hysteresis, and seems to correspond to complete wetting.

This thesis thus makes of a humble attempt to demonstrate the novel features of confined liquid crystals comprising of molecules of different symmetries and reports new structures and phase transition among them, utilizing the power and convenience of Markov chain Monte Carlo techniques.