Simulating Liquid Crystals

Here I present an investigation into the phase behaviour of an exciting new DNA-based liquid crystal system. As well as having direct applications in a new generation of biological liquid crystal display technology, our understanding of the phase behaviour of DNA oligomers fuels the development of DNA nanostructure development.

# Introduction

**Liquid Crystals:** Liquid crystal is used as a broad term to encompass many materials with behaviours between that of conventional liquids and crystalline solids. This is easiest to characterise from a symmetry perspective; crystalline solids display translational and rotational symmetry (i.e. positional and orientational order) through the alignment of particles on a lattice, while liquids do not display any such order. Here we will focus on two particularly common phases, depicted in onscreen.

Firstly, we consider the nematic phase, which displays long range orientational order throughout the sample as all molecules are orientated along the same axis. We may also introduce positional order along one axis to form the smectic phase, leading to layers of similarly alignment molecules, as depicted in the centre of the figure here.

**Phase Transitions:** There are two primary classes of phase transition. Here we will focus solely on lyotropic phase transitions which are driven by changes in concentration, as opposed to temperature driven thermotropic transitions. Furthermore, we consider entropically driven phase transitions where the interaction potentials are purely repulsive. These are an effective benchmark for DNA-based systems; where Debye screening means the potential is almost purely repulsive.

**Order Parameter:** These phase transitions may be defined by an order parameter, which quantifies the degree of order in a given phase and is chosen such that it is non zero in the ordered phase but vanishes in the isotropic phase.

For the nematic order parameter S\_n, we traditionally use the second Legendre polynomial of cos (theta), where theta is the angle between each molecule’s axis and the system director. Similarly, we introduce a smectic order parameter S\_s, to characterise the formation of one-dimensional positional order, by taking Fourier component of the normalised density along the director n, for layers or periodicity L.

**DNA:** Here DNA is used as the basis for the liquid crystal molecules, due to the high specificity with which it can be reliably manufactured and tuned on the nanoscale. These techniques may be applied to developing DNA origami, the process whereby complex nano-structures are constructed out of DNA molecules. Though a greater understanding of the phase behaviour of DNA nanoparticles, we may inform design of more complex structures, and develop colloidal self-assembly processes.

# Methods

**LAMMPS:** I used LAMMPS software

**Nunchuck Molecules:** The simulation molecules considered – use images from Jiamings presentation?

# Rigid Rod Simulations

**Nematic Phase Transition:** We initially consider the nematic phase transition to validate the predictions mate by Onsager theory

**Smectic Phase Transition:** We also consider simulations initiated from a perfectly ordered crystalline phase region, to eliminate the possibility of hysterises in the phase transition, confirming this was a true equilibrium transition. We also were able to identify a continuous (first-order) smectic to nematic phase transition..

# Nunchuck Simulations

**Fived Rigidity:** Initially we configured particles with a variable opening angle limited by the rigidity of the connecting bond, and observed strong evidence for order formation through the formation of a favoured angle distribution throughout the sample. The figure shows the development of this peak in opening angle as the system evolves from the blue **?** lines to the yellow

**Fixed Angle:** To aid ordered phase formation, while also aiming to identifying non-traditional nematic phases, we therefore fixed the opening angle below 180 deg.

**Dynamic Properties:** We may also use this MD approach to investigate the dynamic properties of the system

# Conclusions

**Primary Findings:** In this project I introduced new particles/methods and validates with onsager, then explored new phases..

**Further Work:** More research is required to identify the nature of the phase transition, particularly with larger simulation regions to explore periodic order on longer length scales.