Simulating Liquid Crystals

One sentence introduction, about me and this project. One sentence tagline to convince this is interesting!

# Introduction

**Liquid Crystals:** Liquid crystals is used as a broad term to encompass many materials with behaviour between that of conventional solids and liquids. This is easiest to characterise from a symmetry perspective… *(image on this)*

**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.

**Order Parameter:** These phase transitions may be defined by an order parameter (define this term)

**DNA:** Here DNA is used as the basis for the liquid crystal molecules, due to its specificity etc (and other favourable properties – expand on applications here)

# Methods

**LAMMPS:** I used LAMMPS software

**Nunchuck Molecules:** The simulation molecules considered

# 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.