Simulating Liquid Crystals

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The specificity of DNA base-pair interactions gives considerable functional control in the design of anisotropic nano-particles, enabling the formation of liquid crystal phases. This project aims to study the liquid phase behaviour of such non-conventional liquid crystal molecules, with a particular focus on the novel 'nunchuck' structure - two rigid rods connected via a flexible linker. The Eiser Group have previously considered intra-molecular interaction potentials at the single-nucleotide level for a single DNA nanoparticle, and I am now implementing these potentials in larger, more coarse-grained models of multiple nanoparticles, through open-source software LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator). Such systems are expected to form smectic (layered) phases at high volume fractions. THIS WILL BE EDITED AT THE END

1 Introduction

What are we studying? (brief) Why are we interested? Applications of this! Outline of report

2 Background

2.1 Liquid Crystals

Include known phases etc

2.2 Onsager Theory

Introduce theoretical predictions to be validated later Mathematical derivations may be provided in appendicies

3 Methods

3.1 Simulation - LAMMPS Software

Detail how this works. Include description of natural units conversions etc

3.2 Analysis

Includes custom written python scripts and OVITO freeware. Credit scripts written by other group members.

4 Rigid Rod Simulations

5 Nunchuck Simulations

6 Conclusion

Summarise key results from above, and emphasise their importance Also give limitations of results obtained, and suggest direction for further work

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Appendix A Onsager Theory

Appendix B Netamtic Order Parameter

include theoretical derivation and calculation

Appendix C Code?