Simulating Liquid Crystals

Kit Gallagher *Supervisors: Prof Erika Eiser, Mr Jiaming Yu*

March 21, 2021

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

References

[1]Z. Xing, C. Ness, D. Frenkel, and E. Eiser, "Structural and linear elastic properties of DNA hydrogels by coarse-grained simulation", Macromolecules **52**, 504–512 (2019).

[2]F. Reinitzer, "Beiträge zur kenntniss des cholesterins", Monatshefte für Chemie - Chemical Monthly **9**, 421–441 (1888).

[3]G. Friedel, "Les états mésomorphes de la matière", Annales de Physique **9**, 273–474 (1922).

[4]G. Gray, *Molecular structure and the properties of liquid crystals* (Academic Press, 1962).

[5]G. H. Heilmeier, J. A. Castellano, and L. A. Zanoni, "Guest-host interactions in nematic liquid crystals", Molecular Crystals **8**, 293–304 (1969).

[6]G. Heilmeier, L. Zanoni, and L. Barton, "Dynamic scattering: a new electrooptic effect in certain classes of nematic liquid crystals", Proceedings of the IEEE **56**, 1162–1171 (1968).

[7]P.-G. de Gennes, "Soft matter (nobel lecture)", Angewandte Chemie International Edition in English **31**, 842–845 (1992).

[8]P. de Gennes and J. Prost, *The physics of liquid crystals*, International Series of Monogr (Clarendon Press, 1993).

[9]T. Kato, Y. Hirai, S. Nakaso, and M. Moriyama, "Liquid-crystalline physical gels", Chemical Society Reviews **36**, 1857 (2007).

[10]S. Chandrasekhar, B. K. Sadashiva, and K. A. Suresh, "Liquid crystals of disc-like molecules", Pramana **9**, 471–480 (1977).

[11]L. L. (Lei), "Bowlic and polar liquid crystal polymers", Molecular Crystals and Liquid Crystals Incorporating Nonlinear Optics **155**, 531–538 (1988).

[12]H. Zimmermann, R. Poupko, Z. Luz, and J. Billard, "Pyramidic mesophases", Zeitschrift für Naturforschung A **40**, 149–160 (1985).

[13]J. Malthete and A. Collet, "Liquid crystals with a cone-shaped cyclotriveratrylene core", New Journal of Chemistry (NJC) **9**, 151–153 (1985).

[14]L. Onsager, "The effects of shape on the interaction of colloidal particles", Annals of the New York Academy of Sciences **51**, 627–659 (1949).

[15]M. Doi, S. Edwards, and S. Edwards, *The theory of polymer dynamics*, Comparative Pathobiology - Studies in the Postmodern Theory of Education (Clarendon Press, 1988) Chap. 10, pp. 351–358.

[16]G. T. Stewart, "Liquid crystals in biological systems", Molecular Crystals **1**, 563–580 (1966).

[17]A. D. Rey, E. Herrera-Valencia, and Y. K. Murugesan, "Structure and dynamics of biological liquid crystals", Liquid Crystals **41**, 430–451 (2013).

[18]J. Zhao, U. Gulan, T. Horie, N. Ohmura, J. Han, C. Yang, J. Kong, S. Wang, and B. B. Xu, "Advances in biological liquid crystals", Small **15**, 1900019 (2019).

[19]V. Luzzati and A. Nicolaieff, "Etude par diffusion des rayons x aux petits angles des gels d'acide désoxyribonucléique et de nucléoprotéines : (note préliminaire)", Journal of Molecular Biology **1**, 127–IN5 (1959).

[20]C. Robinson, "Liquid-crystalline structures in polypeptide solutions", Tetrahedron **13**, 219–234 (1961).

[21]T. E. Strzelecka, M. W. Davidson, and R. L. Rill, "Multiple liquid crystal phases of DNA at high concentrations", Nature **331**, 457–460 (1988).

[22]P. Bolhuis and D. Frenkel, "Tracing the phase boundaries of hard spherocylinders", The Journal of Chemical Physics **106**, 666–687 (1997).

[23]M. Nakata, G. Zanchetta, B. D. Chapman, C. D. Jones, J. O. Cross, R. Pindak, T. Bellini, and N. A. Clark, "End-to-end stacking and liquid crystal condensation of 6- to 20-base pair DNA duplexes", Science **318**, 1276–1279 (2007).

[24]G. Zanchetta, M. Nakata, M. Buscaglia, T. Bellini, and N. A. Clark, "Phase separation and liquid crystallization of complementary sequences in mixtures of nanoDNA oligomers", Proceedings of the National Academy of Sciences **105**, 1111–1117 (2008).

[25]S. Nummelin, J. Kommeri, M. A. Kostiainen, and V. Linko, "Evolution of structural DNA nanotechnology", Advanced Materials **30**, 1703721 (2018).

[26]F. Praetorius, B. Kick, K. L. Behler, M. N. Honemann, D. Weuster-Botz, and H. Dietz, "Biotechnological mass production of DNA origami", Nature **552**, 84–87 (2017).

[27]M. Bathe and P. W. Rothemund, "DNA nanotechnology: a foundation for programmable nanoscale materials", MRS Bulletin **42**, 882–888 (2017).

[28]H. I. Ingólfsson, C. A. Lopez, J. J. Uusitalo, D. H. de Jong, S. M. Gopal, X. Periole, and S. J. Marrink, "The power of coarse graining in biomolecular simulations", Wiley Interdisciplinary Reviews: Computational Molecular Science **4**, 225–248 (2013).

[29]D. A. Potoyan, A. Savelyev, and G. A. Papoian, "Recent successes in coarse-grained modeling of DNA", Wiley Interdisciplinary Reviews: Computational Molecular Science **3**, 69–83 (2012).

[30]A. D. MacKerell, J. Wiorkiewicz-Kuczera, and M. Karplus, "An all-atom empirical energy function for the simulation of nucleic acids", Journal of the American Chemical Society **117**, 11946–11975 (1995).

[31]R. Salomon-Ferrer, D. A. Case, and R. C. Walker, "An overview of the amber biomolecular simulation package", Wiley Interdisciplinary Reviews: Computational Molecular Science **3**, 198–210 (2012).

[32]T. E. Cheatham, "Simulation and modelling of nucleic acid structure, dynamics and interactions", Current Opinion in Structural Biology **14**, 360–367 (2004).

[33]D. Michieletto, E. Orlandini, and D. Marenduzzo, "Polymer model with epigenetic recoloring reveals a pathway for the de novo establishment and 3D organization of chromatin domains", Physical Review X **6** (2016).

[34]M. Salamonczyk, J. Zhang, G. Portale, C. Zhu, E. Kentzinger, J. T. Gleeson, A. Jakli, C. D. Michele, J. K. G. Dhont, S. Sprunt, and E. Stiakakis, "Smectic phase in suspensions of gapped DNA duplexes", Nature Communications **7** (2016).

[35]P. Šulc, F. Romano, T. E. Ouldridge, L. Rovigatti, J. P. K. Doye, and A. A. Louis, "Sequence-dependent thermodynamics of a coarse-grained DNA model", The Journal of Chemical Physics **137**, 135101, 135101 (2012).

[36]*Large-scale atomic/molecular massively parallel simulator*, Sandia National Labs, (Mar. 2020) `http://lammps.sandia.gov`.

[37]S. Plimpton, "Fast parallel algorithms for short-range molecular dynamics", Journal of Computational Physics **117**, 1–19 (1995).

[38]H. G. Garcia, P. Grayson, L. Han, M. Inamdar, J. Kondev, P. C. Nelson, R. Phillips, J. Widom, and P. A. Wiggins, "Biological consequences of tightly bent DNA: the other life of a macromolecular celebrity", Biopolymers **85**, 115–130 (2007).

[39]W. Shinoda, M. Shiga, and M. Mikami, "Rapid estimation of elastic constants by molecular dynamics simulation under constant stress", Physical Review B **69**, 10.1103/physrevb.69.134103 (2004).

[40]A. Stukowski, "Visualization and analysis of atomistic simulation data with OVITO–the open visualization tool", Modelling and Simulation in Materials Science and Engineering **18**, 015012 (2009).

Appendix A Onsager Theory

Appendix B Netamtic Order Parameter

include theoretical derivation and calculation

Appendix C Code?