Simulating Liquid Crystals

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The programmability of DNA allows us to design anisotropic nano-particles such as rods, triangles and many other shapes. Such anisotropy is a pre-requisite to form liquid crystalline structures. The exciting part is that because we can now make new shapes we expect to obtain completely new liquid crystalline symmetries. Based on oxDNA, a semi-coarse-grained, freely available simulation package that can provide the topological and stability criteria of any DNA nano-particle, the Eiser group developed a more coarse-grained model to simulate large numbers of these mesogens such that their phase-behavior can be studied.

1 Introduction

In his project the student will use a cours-grained model, based on LAMMPS [1], to study the phase behaviour of 'nunchuks', which are two hard rods connected via a flexible linker, such that they can vary their configuration from fully stretched to folded. Such systems are expected to form smectic (layered) phases at high volume fractions.

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).