Project title	Theory and Simulations of Passive and Active/Living Liquid Crystals
Principal supervisor	Dr. Elsen Tjhung
Second supervisor	Dr. Abdallah Daddi-Moussa-Ider
Discipline	Applied Mathematics and Theoretical Physics
Research area/keywords	Statistical Physics, Fluid Mechanics, and Complex Fluids
Suitable for	Full time applicants, Part time applicants

Project background and description

Liquid crystals are an interesting state of matter with long-range orientational order but without positional order. Consequently these materials can flow like liquids but at the same time, retain an elastic, solid-like response to deformations in their orientational order. The liquid crystal industry is expected to be worth more than 190 billions US dollars by 2023, and yet the technology behind it still relies largely on the nematic phase which was first studied by Leslie, Ericksen and de Gennes *et al.* in the 1960's.

The usual nematic phase in liquid crystals is formed by rod-shaped molecules. At high temperature, the molecules' orientations are completely random [this is called the isotropic phase, see Fig. 1(a) left]. On the other hand at low temperature, the molecules tend to align along some spontaneously broken direction [this is called the nematic phase, see Fig. 1(a) right]. The following youtube video, by my student: https://www.youtube.com/watch?v=dzS7-ddZAzQ demonstrates a simple isotropic-nematic phase transition using just a gas lighter and a laptop screen.

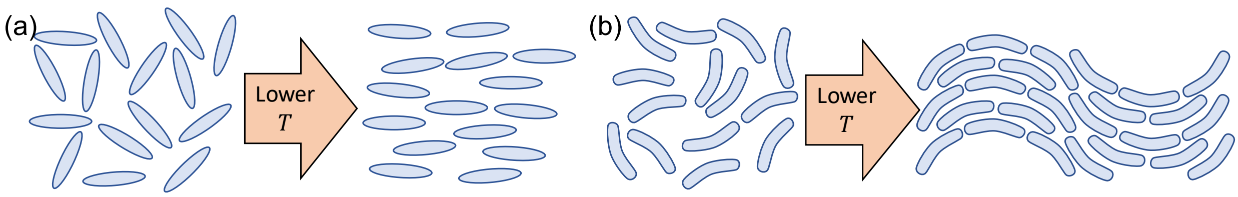

Figure 1: (a) Isotropic to nematic phase transition in rod-shaped molecules. (b) Isotropic to splay-bend phase transition in banana-shaped molecules.

The nematic phase makes up almost all the liquid crystal displays used in our laptops and computer screens. However, many liquid crystalline-forming molecules in nature are not straight. For instance, one can imagine banana-shaped [as depicted in Fig. 1(b)] or cone-shaped molecules. What kind of liquid-crystalline phases do they form? In the case of banana-shaped molecules, at low temperature, the molecules can orient themselves giving rise to a bend modulation, as shown in Fig. 1(b). This new phase is called the splay-bend phase (see Ref. 1). The splay-bend phase is predicted to have some interesting optical properties (such as birefringence) which can make a novel 3D display, without requiring the users to wear any special glasses.

Separately from the above examples, protein filaments such as microtubules and actin filaments inside living cells can also from liquid crystalline order. However, the dynamics of these filaments are far-from-equilibrium, since the filaments are cross-linked by motor proteins, which constantly pull the filaments, and thus doing work on the filaments. In other words, the motor proteins generates an internal and active stress on the fluid, which drives the fluid to be out-of-equilibrium. This active stress can give rise to new physics such as spontaneous flow and negative viscosity, which are not seen in equilibrium liquid crystals.

In this research, we will combine state-of-the-art numerical techniques such as molecular dynamics and lattice Boltzmann with theoretical modelling such as Landau theory and renormalization group to uncover new macroscopic behaviours such as phase transitions, defect formations, and response to external fields.

Background reading/references

- X. Ma and E. Tjhung, Banana- and pizza-slice-shaped mesogens give a new constrained $O(n)$ ferromagnet universality class, *Phys. Rev. E*, **100**, 012701 (2019).
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- T. Markovich, E. Tjhung, and M. E. Cates, Shear-Induced First-Order Transition in Polar Liquid Crystals, *Phys. Rev. Lett.*, **122**, 088004 (2019).
- T. Markovich, E. Tjhung, and M. E. Cates, Chiral active matter: microscopic 'torque dipoles' have more than one hydrodynamic description, *New J. Phys.*, **21**, 112001 (2019).