British Liquid Crystal Society - Annual Conference 2018 – Abstract Book

Oral Presentations

O1. Twisted but never bitter: Spontaneous formation of chiral structures from achiral liquid-crystalline molecules

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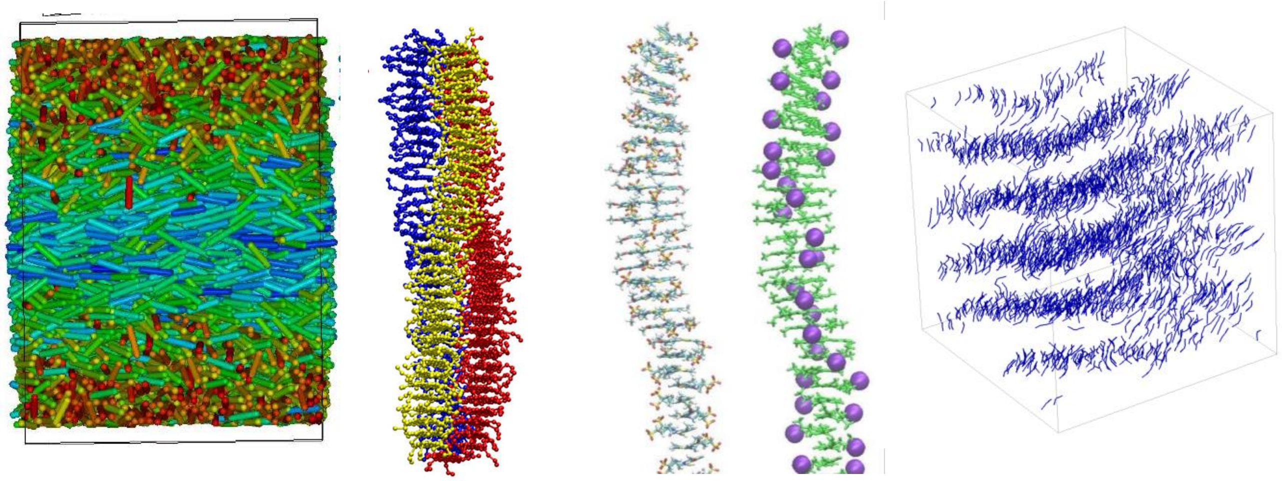
Abstract

Chirality is ubiquitous in liquid crystal systems from chiral phases to the humble twisted nematic display. Back in 1888, Friedrich Reinitzer discovered the first liquid crystal from a derivative of cholesterol [1]. The molecules Reinitzer worked with were chiral (i.e. a molecule and its mirror image are not superimposable), but it turned out that this chirality was transmitted to the whole phase. Hence, the first liquid crystal phase discovered was itself chiral: the cholesteric (chiral nematic) phase.

Intriguingly, liquid crystals can manifest chirality without the molecules themselves being chiral. In fact, under the right conditions, achiral molecules can give rise to chiral structures. This emergent chirality is a fascinating phenomenon and this talk describes our attempts to use computer simulation models to understand what happens in these systems from a molecular viewpoint.

We show examples where achiral bent-core molecules behave as chiral dopants [2-4], where twisted structures arise from cooling bulk nematics [5], where twisted chromonic stacks arise from achiral amphiphiles, and where supramolecular interactions cause complex self-assembly into chiral structures [6].



Snapshots pictures of chiral structures arising from molecular simulations at atomistic and coarse-grained levels.

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O2. Development of coarse-grained models for the simulation of non-ionic chromonic liquid crystals

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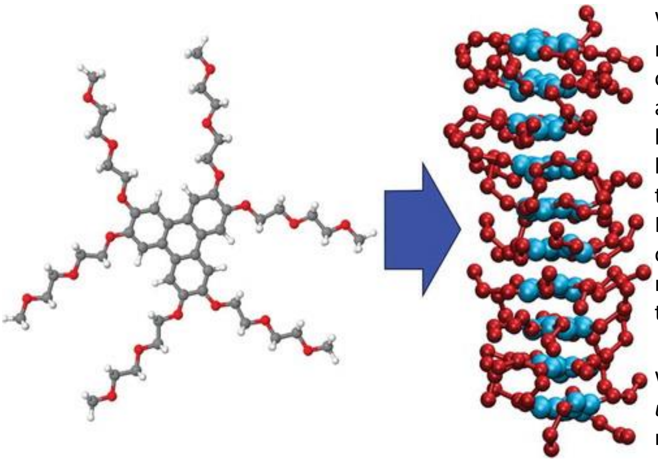
Abstract

Molecular dynamics simulations have been used to gain many significant insights into the behaviour of liquid crystals. Atomistically detailed simulations, however, are limited by the relatively small length- and timescales which are computationally accessible using these models. The use of coarse-grained (CG) models, in which groups of atoms are combined into single interaction sites, could allow larger simulations to be performed, and therefore allow us to probe the behaviour of liquid crystals over larger length- and timescales.

Here, we present investigations into the parametrisation of CG models of the non-ionic chromonic liquid crystal, TP6EO2M, with a view to highlighting the strengths and pitfalls of different coarse-graining methods. We have used both *top-down* (from experimental data) and *bottom-up* (from a reference atomistic simulation) methods in this work.



We have recently shown[1] that two *top-down* coarse-grained models, based on the MARTINI model and the SAFT-γ equation of state respectively, can qualitatively reproduce the formation and structure of chromonic stacks in the non-ionic chromonic liquid crystal, TP6EO2M. The parametrisation of these models has provided insights into which interactions are important to the self-assembly of a chromonic stack over other aggregates. However, there are quantitative differences between the results of the CG models and atomistic simulations and further work is required to obtain models which more quantitatively describe the behaviour of this system.

We also present recent work on the parametrisation of *bottom-up* CG models of TP6EO2M. These models should, in principle, represent an improvement over *top-down* models in reproducing more detailed structural features of the system of interest. However, parametrising these models is a particularly challenging task; the anisotropic nature of liquid crystal structures, combined with the long timescales associated with structural changes, makes an adequate sampling of all distances and orientations in an atomistic simulation very difficult. We describe attempts to parametrise a CG model using the force matching method, and also consider the use of target data more specifically suited to liquid crystals, such as stacking distances.

[1] Thomas D. Potter, Jos Tasche, Elin L. Barrett, Martin Walker & Mark R. Wilson.
Development of new coarse-grained models for chromonic liquid crystals: insights from top-down approaches *Liquid Crystals*, 2017, 12-13, 1979-1989.

O3. Modelling columnar inclusions of stacked rafts in lamellar bodies

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Abstract

Multi-lamellar stacks of phospholipid membranes appear in many living organisms (e.g. in plant chloroplasts). These membranes can be composed of a mixture of saturated and unsaturated phospholipids, and cholesterol. When reduced to sufficient temperature, the mixture separates into liquid-disordered (containing mostly unsaturated lipids) and liquid-ordered (containing higher levels of saturated lipids and cholesterol) phases, which can coexist. [1] It has been observed that these liquid-ordered domains align across the multi-layer system, resulting in columnar ordering of liquid-ordered rafts across many neighbouring membranes. [2]

These stacks of membranes can be naturally modelled as smectic liquid crystals. The nature of the liquid-ordered regions as being relatively static and much less flexible than the surrounding liquid-disordered region, invites us to consider the liquid-ordered region as an inclusion within the smectic. Inclusions such as these can deform the arrangement of layers within the lamellar body by locally fixing the spacing between neighbouring membranes. [3]

We construct a general Hamiltonian for an infinite system, using the Landau de-Gennes Hamiltonian to account for the energy of the bulk. [4] This is used to determine the energy required to form stable liquid-ordered columns in the smectic and so show that columns of the kind observed can be stable, despite their locally distorting the layer spacing of the lamellae.

By exploiting the symmetry of the layer-distortion caused by inclusions, we are able to enforce a periodicity in the model. In then considering only a single period we are able to capture the characteristics of a finite slab geometry within the framework previously constructed.

This model is able to predict many of the properties of aligned liquid-odered phases observed in lamellar stacks. In particular, size of domains relative to the dimensions of the slab, and their preference for certain positions within the stack is captured by our results.

O4. Phase behaviour of colloidal liquid crystals of hard cuboids

***<u>Alessandro Patti</u>*[1]*, Alejandro Cuetos*[2]*, Matthew Dennison*[3]*, Andrew Masters*[1]*, Daniel Corbett*[1]**

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Abstract

We study the phase behaviour of colloidal suspensions of monodisperse and bidisperse hard board-like particles (HBPs) as a function of their shape anisotropy, and observe a fascinating spectrum of nematic, smectic, and columnar liquid-crystalline phases, whose formation is entirely driven by excluded volume effects.

We map out the phase diagram of HBPs by gradually modifying their shape from prolate to oblate and investigate the long-range order of the resulting morphologies along the phase directors and perpendicularly to them. The intrinsic biaxial nature of these particles promotes the formation of positionally ordered biaxial phases, but does not show solid evidence that it would, per se, promote the formation of the biaxial nematic phase. Our simulations shed light on the controversial existence of the discotic smectic phase, whose layers are as thick as the minor particle dimension, which is stable in a relatively large portion of our phase diagrams.

Additionally, we modify the Onsager theory to describe the isotropic-nematic phase transition of freely rotating biaxial particles as a function of the particle width, and find a relatively strong first-order signature, in excellent agreement with our simulations. In an attempt to shed light on the elusive formation of the biaxial nematic phase, we apply this theory to predict the uniaxial-biaxial nematic phase transition and confirm, again in agreement with simulations, the prevailing stability of the positionally ordered smectic phase over the orientationally ordered biaxial nematic phase.

In order to understand the effect of size dispersity on the formation of the biaxial nematic phase, we investigate binary mixtures of short and long HBPs, as previously studied by a mean field theory within the restricted orientation (Zwanzig model). We observe a strong demixing at relatively large density, with an especially stable smectic phase mostly formed by long HBPs at equilibrium with an isotropic phase of mostly short HBPs. Again, no evidence of the nematic biaxial phase is detected. Preliminary simulation results seem to indicate that this behaviour changes when the system is particularly polydisperse.

O5. Manipulating nematic elastomers with light

Daniel Corbett

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Abstract

Long, flexible chains with rods and spacers lead to nematic polymer melts. Crosslinking the chains leads to highly extensible nematic elastomers which combine the molecular fluidity of a rubber with the orientational ordering of a nematic liquid crystal. Nematic elastomers change shape drastically when order is lost, reversible changes of 400% are easy to achieve. If the rods are dye molecules, photons can excite them from a rod-like trans state into a bent cis conformation.

The bent rods reduce the orientational order and the shape of the nematic elastomer in response to heat is duplicated by illumination.

Unlike heat, light penetrates quickly, is easy to deliver remotely, and optical polarisation offers additional control over mechanics. We discuss several novel photo-mechanical effects.

O6. Programming colloidal self-assembly for structural hierarchy

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Abstract

Self-assembly is central to life, which showcases fascinating illustrations of functional organisation, often with remarkable structural hierarchies. Next-generation synthetic materials with structural hierarchies spanning multiple length scales to rival biological complexity are thus much sought-after. While colloidal self-assembly is a promising bottom-up means for structure fabrication [1-2], programming hierarchical schemes for colloidal self-assembly faces the grand challenge of bridging hierarchies of multiple length- and time-scales associated with structure and dynamics along complex self-assembly pathways [3]. In this contribution, I will present our recent work, which explores a generic design principle, exploiting a hierarchy of interaction strengths, to address this challenge *in silico* in close connection with contemporary experimental research [4].

In this work, we employed a variety of computational techniques to realize the generic design principle with triblock patchy colloidal particles and demonstrate their hierarchical self-assembly into two distinct colloidal crystals, each exhibiting a two-level structural hierarchy. In particular, we obtained cubic diamond and body-centered cubic crystals via distinct clusters of uniform size and shape, namely tetrahedra and octahedra, respectively for different designer triblock patchy particles complying with the generic design principle. Our design rules thus addressed a major challenge of assembling colloidal clusters at the first level in a self-limiting way for them to serve as uniform secondary building blocks for the next level of assembly [5]. Such a conceptual design framework opens up the prospects of pushing the frontiers colloidal self-assembly. Moreover, the design framework underpins a novel bottom-up route to much sough-after cubic diamond colloidal crystals with attractive photonic applications.

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O7. Shape segregation in molecular organisation: MD simulations and X-ray scattering

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Abstract

The positional order and orientational order exhibited by molecules in smectic phases give rise to materials lending themselves to a range of applications. As a result, much research has focused on structure-property relationships of smectic mesogens in order to develop materials with favourable properties for their suggested applications. One particular area of focus has been on molecules with bulky end-groups; such groups have been reported to promote a range of effects, such as stabilising or destabilising smectic phases, weakening or strengthening interlayer interactions, and stabilising or destabilising the smectic A phase relative to the smectic C phase, depending on the size and chemical composition of the end-group in question, and on the structure of the mesogen.

Siloxane groups have been relatively widely studied in this context, and siloxane-terminated cyanobiphenyls have been shown to exhibit favourable properties for use in scattering devices.[1] Their properties are typically attributed to chemical incompatibility introduced by the siloxane moieties, but recent studies have indicated that similar properties may be exhibited by introducing bulky alkyl substituents,[2,3] suggesting that chemical incompatibility may not be the cause of the differences in material properties.

We have carried out experimental and computational studies on the cyanobiphenyl molecules shown in Figure 1. X-ray scattering studies enabled smectic layer spacings and translational order parameters to be determined, and the experimental trends were matched by those calculated from fully atomistic MD simulations. The degrees of molecular interdigitation in the simulations were quantified and related to the sizes of the terminal groups, suggesting that "shape segregation" gives rise to significantly different layer structures between the two materials. The atomic resolution results from the MD simulations provide a data-set from which results of experimental X-ray mesurements may be understood and rationalised.

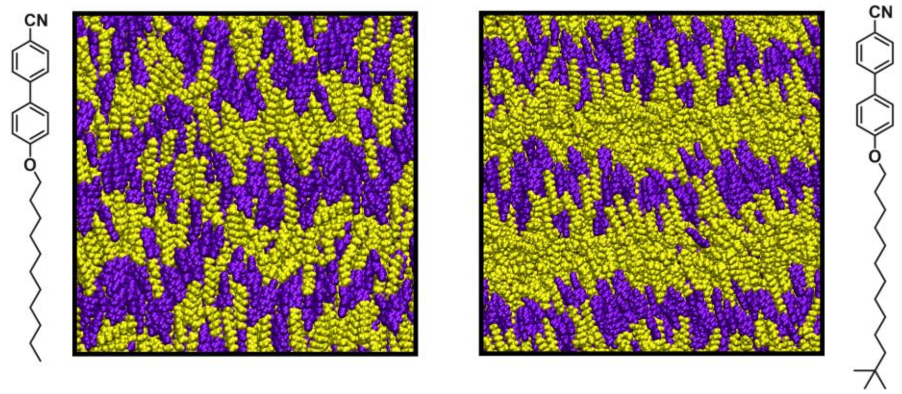

Figure 1 Structures of the two molecules studied in this work (far left and right) along with snapshots of the MD simulations (middle left and right) with the aromatic and aliphatic regions coloured in purple and yellow, respectively.

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O8. Studying sanidic lamellar-like mesophases in conjugated polymers using a new symmetry-inspired model

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Abstract

In conjugated polymers, charge transport properties are known to be strongly affected by morphology. An interesting recent observation is that, to achieve high mobilities, perfect lamellar order is not necessary [1]. Here we present a simple model that enables the study of sanidic liquid crystalline mesophases characterized by partial lamellar order, at device-relevant length scales. Nonbonded interactions responsible for coplanarity in chain orientation and for stacking are described by anisotropic soft potentials constructed on the basis of simple symmetry considerations. Using polyalkylthiophenes as a test system, we perform Monte Carlo simulations of chains of various lengths. Lamellar-like morphologies are obtained, either as mono- or poly-domains. The type of lamellar order is identified by computing 2D scattering patterns, which can be compared with experimental GIWAXS data. From this analysis, we conclude that our morphologies indeed reproduce an experimentaly reported liquid crystalline mesophase [2]. We analyze the organization of chains inside the lamellae and identify in a simple way connectivity pathways between lamellae. In the future, atomistic details can be reintroduced via backmapping, allowing for prediction of charge transport properties [3].

References:
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O9. Nematic liquid crystal director structures in rectangular regions

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Abstract

Interest in the confinement of liquid crystals between solid boundaries originally came about out of necessity, viewing a liquid crystal under a microscope was only possible if this liquid was held in place by at least one solid boundary. Later it became clear that the competition between the orientational influence of a solid boundary and the influence of internal effects such as elasticity or external effects such as an applied electric field could lead to interesting effects of both scientific and technological interest.

We consider confinement of a nematic liquid crystal in a shallow rectangular well subject to weak anchoring on the sides of the well. By considering weak planar anchoring instead of infinitely strong anchoring, we are able to analyse nematic equilibria in the well without the need to exclude point defects at the corners. We employ the standard one-constant approximation for the Frank elastic constants and a Rapini-Papoular surface energy to model the weak anchoring effects. By minimising the total free energy, we are able to derive an equation for the director angle. The derived system permits two undistorted states, and we find four multistable distorted states bifurcating from these constant states, at some critical anchoring strength. The critical anchoring strength at which these distorted states occur will vary depending on the aspect ratio of the rectangular well. Each of these four states have different optical properties and energies. We find that in the limit of large anchoring strength, there are similarities between our approach and the infinitely strong anchoring approach.

O10. Deformation and chaining of flexible shells in a nematic solvent

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Abstract

A micrometer-scale elastic shell immersed in a nematic liquid crystal may be deformed by the host if the cost of deformation is comparable to the cost of elastic deformation of the nematic. Moreover, such inclusions interact and form chains due to quadrupolar distortions induced in the host. A continuum theory model using finite elements is developed for this system, using mesh regularization and dynamic refinement to ensure quality of the numerical representation even for large deformations. From this model, we determine the influence of the shell elasticity, nematic elasticity and anchoring condition on the shape of the shell and hence extract parameter values from an experimental realization. Extending the model to multi-body interactions, we predict the alignment angle of the chain with respect to the host nematic as a function of aspect ratio, which is found to be in excellent agreement with experiments and greatly improves upon previous theoretical predictions.

O11. Chiral nematic liquid crystals in torus-shaped and cylindrical cavities

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Abstract

The topological properties of ordered fluids such as nematic liquid crystals in confined geometries have received considerable attention in the past few decades because of the rich behaviour that results from the frustration between the elastic energy of the bulk and surface energy imposed at the interface. Here we investigate nematic and chiral nematic phases confined within cylindrical and torus-shaped cavities with both planar and homeotropic anchoring using computer simulations.

We have performed Monte Carlo simulations using a coarse-grained model based on hard spheres with an embedded orientational unit vector which has previously been used to investigate nematic shells [1]. For systems with planar degenerate anchoring, we find a defect-free ground state, in agreement with the Poincaré-Hopf theorem [2] which states that the total topological defect charge at a surface is equal to the Euler characteristic, *i.e.* zero for cylindrical and torus-shaped cavities.

For non-chiral nematic systems with homeotropic anchoring, we find a pair of s=+1/2 disclination lines parallel to the tube axis that, in the case of a torus, form closed loops around the major circumference of the torus. As the chirality increases we find that the helical pitch causes the disclination lines to twist, forming helical arrangements in cylindrical cavities. In a toroidal cavity the amount of twist (n) in the director field when travelling around the major circumference is necessarily a multiple of half integer twists so that the director is continuous. This leads to the disclinations forming torus knots or torus links (Figure 1), depending on whether the total twist is half integer or integer. In the case of half integers, a single disclination line is formed, which encircles the cavity twice before joining to itself, producing torus knot structures such as the trefoil (n=1.5) and cinquefoil (n=2.5) knots. In contrast, when n is integer, two distinct disclination lines form [3].

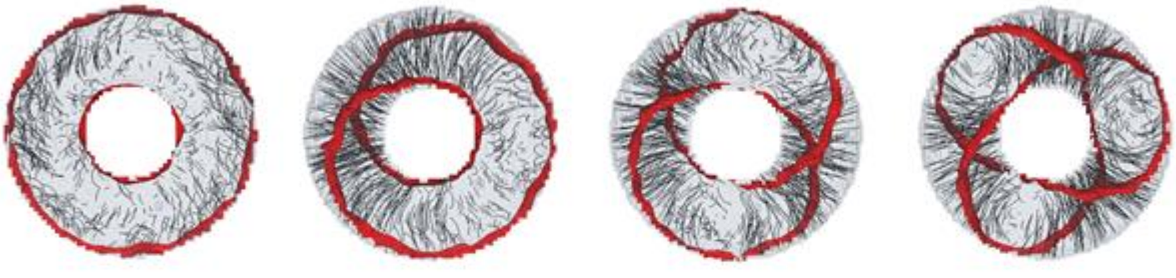

Figure 1 Examples of defect configurations observed in chiral nematic tori with homeotropic anchoring forming two loops separate loops, one loop, two interlinked loops and a trefoil knot. The chirality increases from left to right.

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O12. Two-dimensional blue phases and controllable cholesteric membrane shapes

***Luuk Metselaar*, Amin Doostmohammadi, Julia M. Yeomans**

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Abstract

Recent experiments by Nych et al. [1] showed the first direct optical observation of half-skyrmions in a thin film of chiral nematic liquid crystal. We provide fully dynamical simulations of the transition from the two-dimensional isotropic phase to the two-dimensional cholesteric and blue phases, characterised by the emergence of half-skyrmions.

Building on these findings, we confine the cholesteric and blue phases to a finite-sized membrane and show a wealth of membrane shapes, ranging from circular to star-shaped, based on the characteristic pitch of the cholesteric.

We further show that by applying external fields we are able to dynamically control the membrane shapes. A strong enough field perpendicular to the membrane will for instance lead to a configuration observed in membranes of fd-virus [2], with a homogeneous director field in the middle of the membrane, but twisting at the edges. Releasing the membrane again leads to the possibility of reconfigurable membrane shapes by subsequent application of different fields.

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O13. The role of elasticity in nematic Poiseuille flow under electric fields

***Akhshay Bhadwal*[1], *Carl Brown*[1], *Ian Sage*[1], *Andrew Edwards*[1], *Nigel Mottram*[2], *Geoff McKay*[2], *Rachel Tuffin*[3]**

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Abstract

During Poiseuille flow of a layer of nematic liquid crystal the spatially dependent orientation of the nematic director and the velocity profile are determined by number of factors. These include the relative strength and direction of surface anchoring, the flow rate, the relative magnitude of the anisotropic viscous and elastic forces, and the strength of an externally applied electric field orthogonal to the flow direction. The study of such electro-rheological effects in nematics has previously been limited to thick layers, for which elastic forces can be neglected [1][2], and to specific geometries and flow switching phenomena in thinner layers [3].

We report experiments, theoretical analysis, and simulations that elucidate the complex nature of surface-flow-field-director coupling for a thin homogenous nematic layer. For our thin 20 µm layer the surface coupling and elastic forces can significantly affect the stability of the different equilibrium director distortion modes associated with the Fréedericksz transition bifurcation diagram under the influence of flow. In analogy to the sin (*npz*/*d*) director distortion modes in a zero flow classic Fréedericksz transition perturbation analysis, we label these modes *n* = 0, 1, 2.

Our preliminary experimental results demonstrate how externally driven and controlled Poiseuille flow can extend the *n* = 0 branch, for which there is little director distortion. This branch remains metastable, delaying the Fréedericksz transition to voltages even significantly above $2V_C$, where V_C is the Fréedericksz transition voltage in the absence of flow. We find that it is possible to switch between the flow stabilized *n* = 0 branch and the *n* = 1 branch of distorted director configurations via abrupt removal and re-application of externally driven flow. Furthermore, we find that a significant hysteresis behaviour is exhibited by *n* = 1 branch around V_c, with width of the hysteresis being determined by the flow rate. These observations are consistent with the results of our numerical bifurcation analysis (performed using the MATCONT Matlab continuation package) of the stability of different modes under flow. Numerical simulations using the Ericksen-Leslie dynamic equations for nematics equations demonstrate the influence the competition between flow and field induced n-director reorientation on the dynamic behavior of the low distortion *n* = 0 mode.

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O14. Liquid Crystal Elastomer Particles: Actuation from Confinement

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Abstract

Liquid crystal elastomers (LCEs) possess a number of properties that make them good candidates for such uses as artificial muscles[1,2], microfluidic valves[3] or chemical sensors[4] because, principally, aligned LCEs contract in the direction parallel to the director on the loss of nematic order. The necessary alignment in films of LCE is typically achieved by polymerisation in a stretched state, however the size of microparticles make this challenging. Through a combination of spherical confinement and alignment conditions it is possible to produce a variety of director configurations, such as bipolar, concentric and radial, in a droplet.[5]

Where actuating LCE particles have previously been prepared by microfluidics a concentric alignment has been achieved by both shear and flow.[2,7-9] To avoid shear influencing the alignment we used a microfluidic strategy that involved a solvent evaporation step, leading to the host PVA/water inducing a bipolar alignment in the droplets. Remarkably, we observed this alignment to be largely maintained during network formation allowing for the preparation of bipolar actuating LCE particles. Our experiments also revealed that a good monodispersity of particles and self-assembly into monolayers can be achieved.

The synthesis and fabrication of aligned nematic elastomer microparticles from laterally-attached nematic monomers is discussed.[10] Control over the actuation temperature and extent of the shape change is also demonstrated. The extent of actuation is comparable to previous attempts; verifying the degree of alignment and, therefore, validity of this approach.

O15. Liquid crystal-ferrofluid dispersions as microscopic viscosity probes

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Abstract

Liquid crystals, as well as colloid science, has long been a topic of interest not only for fundamental studies, but especially also for applications. Besides the discovery of thermotropic phases in 1888 by Reinitzer and Lehmann, already about one century ago it was also realized that colloidal particles themselves can form self-organized phases in the presence of an isotropic liquid solvent[1], so called colloidal lyotropic phases, which were described for example by Freundlich in 1915 for colloidal vanadium pentoxide (V_2O_5) in water. While thermotropic liquid crystals are generally described via dispersion interactions of the Maier-Saupe type, lyotropic colloidal liquid crystals are described by a theory developed originally by Lars Onsager, based on excluded volume. More recently, suspensions of colloidal particles in thermotropic liquid crystals have attracted increasing interest in order to add functionality, tune LC properties, or to use the self-organization as a vehicle to order anisotropic colloidal particles[2].

Following similar initial experiments by Poulin et al.[3], we intend to carry this concept one step further, by suspending anisotropic magnetic particles in an isotropic host, which in turn is then dispersed in a thermotropic nematic liquid crystal. Dispersions of oil based and water based ferrofluids in isotropic liquids (water, glycerine and silicon oil) and liquid crystals (5CB), respectively, were produced at different ferrofluid droplet sizes. Application of magnetic fields causes the ferrofluid droplets to move at a constant terminal speed. A model, based on Stokes' Law with a droplet boundary layer was developed and employed to calculate the carrier fluid viscosity. The model was tested against the known viscosities of the isotropic carrier fluids, and a boundary layer thickness of 4 micrometers could be determined, which conforms very well with the fact that droplets of diameters smaller than approximately 8 micrometers are not observed to display any motion, while generally, larger droplets move faster than smaller ones.

The technique was then applied to the nematic phase of 5CB, one of the most detailed studied liquid crystals available. The terminal velocities for motion along and perpendicular to the director were measured, and the viscosities, as well as the viscosity anisotropy determined. Values correspond well with those determined by macroscopic techniques[4], as does the temperature dependence of the viscosity.

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O16. Side-chain liquid crystal polymers containing acid groups as ionic conductors for low temperature fuel cells

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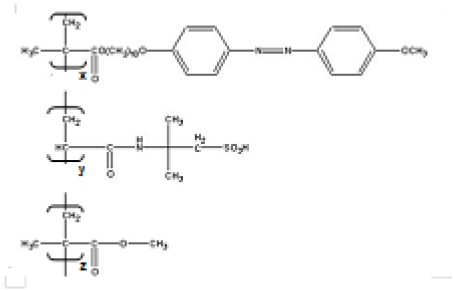
Abstract

The microstructure of efficient electrolytes for electrochemical devices must simultaneously provide with high and selective ionic conductivity while guarantee mechanical and chemical stability[1]. Liquid crystals are excellent candidates as components in low temperature electrolytes due to their ability to form anisotropic morphologies, which can ultimately facilitate the creation of preferred ionic pathways[2]. Moreover, their sensitivity to external stimuli, such as electrical-magnetic fields, mechanical solicitations or light, makes them particularly attractive where a dynamic response is needed[3]. This work discusses the synthesis, physical characterisation and conductivity of a series of side-chain liquid crystal copolymers, the poly[10-(4-methoxyazobenzene - 4'-oxy)decyl methacrylate]-co-poly[2-acrylamido-2-methyl-1-propanesulfonic acid]-co-poly[methylmethacrylate]s, see **Scheme 1**, with potential application as electrolyte components in low temperature fuel cells.



Scheme 1. 10-MeOAzB/AMPS/MMA terpolymers.

The terpolymers were synthesised by one-pot conventional radical polymerisation, and exhibit smectic phases in broad ranges of compositions and molecular weights. While the azobenzene units provide the materials with liquid crystalline and photoresponsive behaviour, the sulfonic groups act as polar sites to promote ion conductivity. The presence and concentration of non-mesogenic/non-ionic methylmethacrylate untits, on the other hand, regulates their structure *via* disruption of the anisotropic and polar interactions. 10-MeOAzB/AMPS/MMA polymers near equimolar compositions show considerable conductivity, and our dielectric results suggest that ion hopping can be activated by local motions in polar regions confined within smectic layers[4], thus controlled by their liquid crystallinity.

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O17. The synthesis and investigation of macro-chiral liquid crystal nanoparticles

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Abstract

Metal nanoparticle (NP) functionalized LC materials are attracting considerable attention due to their potential applications in magnetic, optical and electronic devices. The optical properties of these NPs are often related to the 2D and 3D organisation of such materials. Research on the organic groups for such systems has in the past concentrated mainly on the type of the mesogenic groups selected and to some extend on the functional groups linking the NPs and the mesogens. Chiral group functionalized NPs have been studied for mixtures in LC systems for the induction of chiral phase behaviour in nematic hosts and to a lesser extend for the formation of chiral LC structures. [1, 2] The question, whether LC and chiral group functionalized NPs can modify and amplify the chirality of organic ligands in composition with LC hosts has not been explored in detail. [3] Here we report the results of the synthesis of gold NPs in the size regime from 3-5 nm functionalized with ligands based on the binaphthol motif and with nematogenic groups. [4] The materials were characterised chemically and the ratios between chiral groups and LC groups was determined. The LC properties were determined by optical polarizing microscopy (OPM) and differential scanning calorimetry (DSC) and by synchrotron based XRD studies. Based on these results, phase diagrams with nematic hosts were constructed. For a number of selected mixtures the helical twisting power (htp) of these systems in nematic hosts was determined. The experimental data shows that the htp of the designed chiral_LC_Au_NPs is significantly larger than that of the chiral groups dispersed in the LC host and larger than that of NPs functionalized only with chiral groups. The properties of these systems will be discussed and will be compared to structurally related materials.

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O18. Reactive mesogens: One principle - infinite possibilities

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Abstract

Since their development in the 80's of last century, reactive mesogens (RM's) form a versatile class of soft matter materials that have find their way to a wealth of applications. The frozen-in molecular order of the polymer networks that they form upon polymerization brought a new dimension into liquid crystal technologies. Initially developed for their use as low shrinkage, low thermal stress coatings, the RM's demonstrated their function especially in optical applications. The large, temperature-stable and adjustable birefringence was adopted by the display industry for many purposes, varying from viewing angle enhancement to optical-retarder based 3D imaging optics. Presently, advanced optical applications for augmented reality and astronomy lenses are drawing much attention as well as their use to stabilize special liquid crystal effects for smart windows and dedicated display types.

The use of RM's for soft robotics applications is nowadays studied by many academic and industrial institutes. Triggered by heat, light or humidity the polymers change shape, surface structure or porosity. At Eindhoven University, we developed self-sustaining oscillators, cilia based micro-transport devices and haptic surfaces. Films deform from a flat to a complex, but pre-designed, shape with prospects to light-triggered origami and self-folding plastic elements. A completely new development relates to coatings that switch their surfaces from flat to corrugated with a preset topography. Or in a different design from dry to wet by controlled

secretion of liquid. Properties that enable controlling properties as friction, grip, lubrication, stick, soil rejection, particle manipulation, etc.

The lecture will discuss part of the history next to our newest developments in responsive liquid crystal polymer materials, giving a preliminary view on the future of RM's with advanced applications in the fields of oscillatory films, smart coatings, soft robotics and haptics.

O19. Enhanced smectic A stability in rod-like materials by incorporating cyclic end groups

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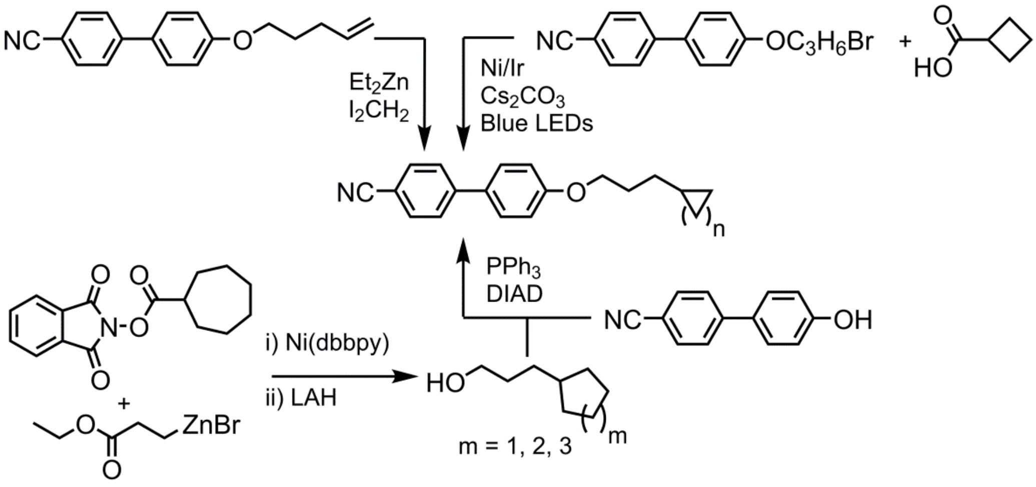
Abstract

In recent years there has been renewed interest in smectic A scattering devices due to simpler device construction and bistable operation. While engineering low melting points *via* terminal groups such as siloxanes is trivial [1] these are typically also detrimental to the stability of the smectic A phase; we therefore sought a new method for enhancing smectic A phase stability.

Our initial hit was the unexpected observation that appending a cyclopentyl group to 3OCB leads to an increase in clearing point from 40 °C to 75 °C. To study this phenomenon further we prepared a small library of alkoxy cyanobiphenyls bearing a cyclic terminal group (Figure **1**), varying the size of the terminal ring as well as the length of the spacer connecting the mesogenic unit through decarboxylative sp^3-sp^3 coupling reactions. Large terminal rings (cyclohexyl, cycloheptyl) are found to induce smectic A phases even with short (C3) spacers. Increasing the length of the spacer also leads to an increased tendency to form SmA phases, as well as anomalously large smectic layer spacings.



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O20. Examining the effect of anchoring strength on bistability in liquid crystal displays

***<u>Sophie Jones</u>*[1]*, Guy Bryan-Brown*[2]*, David Walker*[2]*, F Anibal Fernandez*[3]*, Sally Day*[3]*, J Cliff Jones*[1]

[1]University of Leeds, Leeds, United Kingdom. [2]Displaydata Ltd, Malvern, United Kingdom. [3]University College, London, United Kingdom

Abstract

Surface anchoring governs aspects of switching behavior in many liquid crystal displays (LCD) and it is critical for bistable LCDs such as the zenithal bistable display (ZBD) [1,2]. ZBD uses homeotropic anchoring on a deep grating to induce surface bistability. The strength of this anchoring is critical to ZBD latching behaviour and bistability, and so the device produces a means for determining what is a difficult surface property to measure. The effect of the anchoring energy will be investigated through both numerical modelling and experiment for ZBD.

The two stable director alignments ZBD supports are a low-tilt Defect state, with +/-1/2 defects at the top and bottom of the grating grooves, and a near-vertical Continuous state. Either state is selected via flexoelectric switching. Initially, ZBD cells were filled with 4-cyano-4'-pentylbiphenyl (5CB) and latched using bipolar pulse waveforms. The latching thresholds were found, and using the theoretical descriptions of the device and flexoelectric latching, the anchoring strength at the grating surface was determined [3,4]. This was done first for the commercial device's homeotropic-anchoring photopolymer [Fig 1]. Following this, tests were done using a silane surfactant deposited in the vapour phase onto a grating formed in a conventional photopolymer. This treatment method allowed control of the surface density for the surfactant and hence the homeotropic anchoring energy. The electro-optic results are compared with numerical modeling [5] and used to probe the limits of bistability in different device configurations.

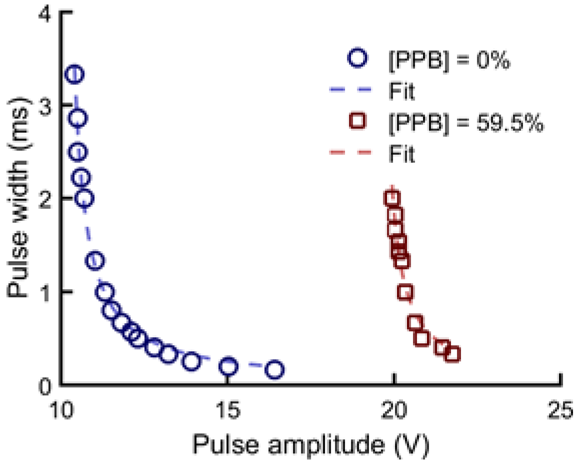

Figure 1: Experimental results with fitted curves for two compositions of the commercial photopolymer gratings

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O21. Grating aligned ferroelectric liquid crystals for use in fast switching devices

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Abstract

Ferroelectric liquid crystals (FLCs) dominated liquid crystal research in the 90's and led to many applications, such as the surface stabilized FLC device [1]. Such a device enables ultra-fast optical response times of under 200 µs [2]. Unfortunately they are sensitive to shock induced flow, whereby the smectic layers are permanently displaced. The prospect of novel alignment geometries has reopened the interest in FLCs for fast switching device applications [3].

This work presents a novel alignment system for FLCs, achieved by the combination of a sinusoidal-like grating with micron-sized features and homeotropic surface treatment. This surface treatment aligns the smectic layers parallel to the substrate, while the grating aligns the c-director perpendicular to the grating vector (Figure 1a). Using an in-plane electric field applied at 45° to the grating vector, the c-director switches to align perpendicular to the field and satisfy the half-wave plate condition (Figure 1b).

This design aims to remove the formation of defects following a shock to the aligned FLC, while maintain ultra-fast response times. An alignment that can be shown to "self-heal" when addressed fixes the difficulties experienced with the SSFLC geometry. This enables many practical display or device applications, such as high frame rate displays and frame sequential colour. In addition we aim to apply this concept to more complex systems, such as the spontaneously ferroelectric bent-core liquid crystals. We aim to fabricate a design that exploits their exciting properties with the potential of yet faster switching modes.

O22. Optical multi-parameter analyser for liquid crystal materials and composites

***Giampaolo D'Alessandro*, Malgosia Kaczmarek, Nina Podoliak**

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Abstract

The performance of liquid crystal devices is determined by a large number of parameters. Some are intrinsic properties of the liquid crystal, either in pure form or as a colloidal suspension: typically these are the elastic constants and the viscosity coefficients. Others characterise the interaction between the liquid crystals and the surfaces that contain them: examples are the anchoring energy and the pretilt angle. Moreover, a device may not just comprise liquid crystals, but also optical active layers that change their electrical or alignment properties as a function of the incident light intensity and frequency. For such devices, the layer parameters, e.g. the photo-conductivity, affect the liquid crystal alignment and, hence, their response. Finally, the parameter of interest may be the long-term stability of the suspension in contact with the other device components.

In all these cases, it is essential to capture an "integrated" response of the whole liquid crystal device and determine its core parameters, ideally measured quickly, accurately and in a reproducible manner over a long time scale.

We have developed an experimental and modelling procedure to do provide such a snapshot of a liquid crystal cell with its alignment layers and have built a self-contained, portable prototype, the Optical Multi-Parameter Analyser (OMPA). Its performance was tested for planar, nematic liquid crystal cells. The idea at the heart of the device is to perform cross-polarised transmission intensity measurements across the whole device area as a function of the frequency and amplitude of the voltage applied to the cell. The data are then fitted using a comprehensive Ericksen-Leslie model to determine the device and liquid crystal parameters. Point-wise measurements of the cross-polarised intensity give us the elastic constants, the pretilt angle, the cell thickness and a set of Leslie viscosities. OMPA collects data from across the cell, which allows us to draw maps of the cell thickness and of the pretilt angle. It also allows us to use a statistical bootstrapping technique to obtain reliable confidence intervals for the liquid crystal parameters. The OMPA can also analyse the response of photosensitive and photoactive layers: for example, in the case of photo-conducting layers, we have been able to measure the relative impedances of the polymer and liquid crystal layers as a function of the incident light intensity. Finally, reliable measurements are obtained for typical, standard liquid crystal cells, without the need for bespoke design, so it is easy to monitor their long term stability and quality. This is particularly important for colloidal suspensions, where phase separation or adsorption at the surface is possible.

O23. PAAD films for reversible photo-aligned liquid crystal devices

Jordan Gill, Elena Perivolari, Nina Podoliak, Giampaolo D'Alessando, Malgosia Kaczmarek

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Abstract

Our work concerns the creation of an optically controlled, rewritable half-wave plate based on a twisted nematic liquid crystal cell. The cell is bistable and switchable, operating in the twist and untwist states (on/off), with the switching between states controlled remotely by the illumination of a PAAD-22D alignment layer with an external light source. PAAD materials are photo-aligning, meaning that their molecules obtain a collective preferred orientation upon exposure to polarised light. This induces a preferred surface orientation in the liquid crystal; specifically, one that is perpendicular to the polarisation of the pump beam. As a result, manipulating the pump polarisation makes reversible switching between the two alignment states at the cell surface possible. Using a blue (405nm) or green (543nm) pump beam, the changes in transmission for probe beam wavelengths covering the visible spectra and near infrared regions are observed. We demonstrate a reproducible modulation of the transmitted polarisation with an efficiency between 90% and 70% in the twist and untwist states.

To better model and improve such rewritable systems utilising PAAD, a good understanding of the dynamics and behaviour of these alignment layers is necessary. Unfortunately, there is little information about the intrinsic optical properties of the PAAD itself, even though it has seen extensive use in liquid crystal photo-alignment. As such, we also present a study of the photo-alignment behaviour of thin PAAD films with visible light. This is done in comparison with experimental work on the diffraction efficiency of photo-induced refractive index gratings formed in thin PAAD layers. We demonstrate that the current photo-alignment model, in which the PAAD aligns perpendicular to the polarisation of the pump beam, does not explain the experimental observations, and a new model to describe the photo-alignment is developed.

O24. Self-assembly of phase amplitude gratings in liquid crystal devices through electro-convection.

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Abstract

The potential for liquid crystals to be used as Spatial Light Modulators (SLMs) has been rapidly developed in recent years, particularly through the development of patterned electrodes to create changeable phase structures. A limitation of patterned electrode techniques, is the resolution of the phase grated structure, being determined in the fabrication process, and cannot be changed in situ.

Electro-convection can refer to a broad range of mechanisms, where liquid crystals can self-assemble into convective rolls through the application of an electric field. These rolls can then be used as a periodic phase grating, for beam steering applications [1]. The formation of these rolls and their properties are determined by a huge number of device characteristics (electronic, viscosity, alignment, applied electric field, thickness etc), but are all principally driven by conduction of ions within the material [2]. The simplest device configuration that exhibits electro-convective behaviour, uses a liquid crystal with negative dielectric anisotropy ($\Delta\varepsilon<0$) and positive conductive anisotropy ($\Delta\sigma>0$) in a planar aligned cell, with a voltage applied across the device (fig 2). At low frequencies, where conduction is possible, the threshold voltage (U) can be described by equation [2]:

$$U(q,f) = \frac{\pi^2 K^{eff}}{\varepsilon_0 \Delta\varepsilon^{eff} + I_h \dfrac{\left(\dfrac{\alpha_3}{q^2} - \alpha_2\right)\tau_q \Delta\sigma^{eff}}{\eta^{eff}}}$$

where f is frequency of a sinusoidal waveform and q is the rolls' wave number. K^{eff}, $\varepsilon_0\Delta\varepsilon^{eff}$, $\Delta\sigma^{eff}$ and η^{eff} are the effective; elastic constant, dielectric anisotropy, conductive anisotropy and viscosity as functions of q and f. τ_q is a charge relaxation time, and α_2 and α_3 are the materials Leslie coefficients. I_h is a constant.

The nature of electro-convection in a calamitic liquid crystal material is presented and the enhancement effect through the addition of electrolytes investigated. The influence of the electrolytes on electro-convective behaviour, will be quantified using dielectric spectroscopy, pitch measurements and diffraction efficiency measurements.

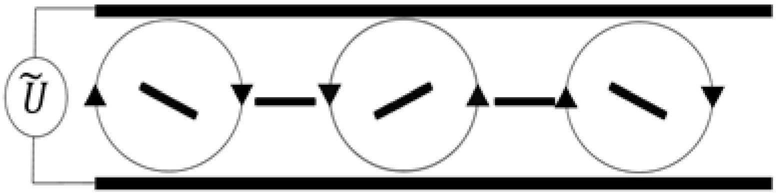

Figure 1: Schematic describing how electro-convection can lead to a periodic phase grating due to director distortion.

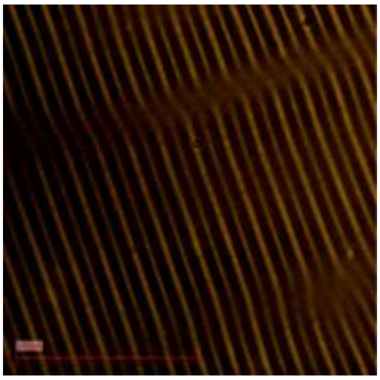

Figure 2: Example of rolls in MLC 2081 with dopant of TBTPB.

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O25. Stay Curious - A story of curiosity and serendipity on the 50th anniversary of liquid crystal research in Merck

Dr Owen Lozman FRSC

Vice President at M Ventures and Head of the Performance Materials Venture Fund

As an undergraduate I was immediately smitten with the amazing richness and diversity of the liquid crystal field and can clearly remember the mixture of wonder and bafflement I experienced at my first BLCS. At the time I was an undergraduate in Leeds, about to embark on a PhD project in Discotic Liquid Crystals. Since then I have had a varied career in R&D before moving into venture capital. I have had the privilege to work with some of the best companies and academics in the field. Along this journey I have also had the pleasure to work with some of Ben Sturgeons colleagues and in sharing some of the new technologies, which Merck is exploring, I will show that Ben's spirit lives on in. The industrial R&D teams and our academic partners continue to invest, invent and persevere to deliver disruptive technologies to the market.

In the year that commercial liquid crystal display research in Merck celebrates its golden anniversary; I will show that there is a still a lot of room for differentiation and innovation both in displays and non-display applications of liquid crystals and that liquid crystalline materials still hold the same combination of fascination and mystery as they did back in my undergraduate days.

As well as sharing my personal experiences of working in the field, I will also explain some of the currently active projects where control of chemistry and phase behaviour yield commercially exploitable phenomenon and how Merck and M Ventures are working together to foster innovation and develop new commercial applications for the amazing materials which simultaneously pay our bills, fill us with wonder and keep us awake at night!

O26. Chirality and the twist-bend nematic phase

__Rebecca Walker__[1], Damian Pociecha[2], Ewa Gorecka[2], John Storey[1], Corrie Imrie[1]

[1]University of Aberdeen, Aberdeen, United Kingdom. [2]University of Warsaw, Warsaw, Poland

Abstract

Following its prediction by Dozov [1], and subsequent experimental identification by Cestari *et al.* [2] the twist-bend nematic phase, N_{TB}, has triggered a resurgence of research interest in the structure-property relationships of liquid crystal dimers. In the N_{TB} phase, the director exhibits periodic twist and maps out a helix with doubly degenerate domains having opposite handedness – giving local spontaneous chirality but an overall achiral phase. The director is tilted at a constant angle ϑ with respect to the helical axis z.

Since the heliconical structure of the N_{TB} phase is not related to molecular chirality, the question arises: what effect does molecular chirality have on the heliconical structure? A transition from the chiral nematic phase to a twist-bend nematic phase has been seen in mixtures with a chiral dopant [3] and the first example of a single molecule showing the N^*_{TB} phase was recently reported in materials containing a cholesterol moiety connected to an azobenzene or Schiff base unit by an odd-membered spacer. [4, 5]

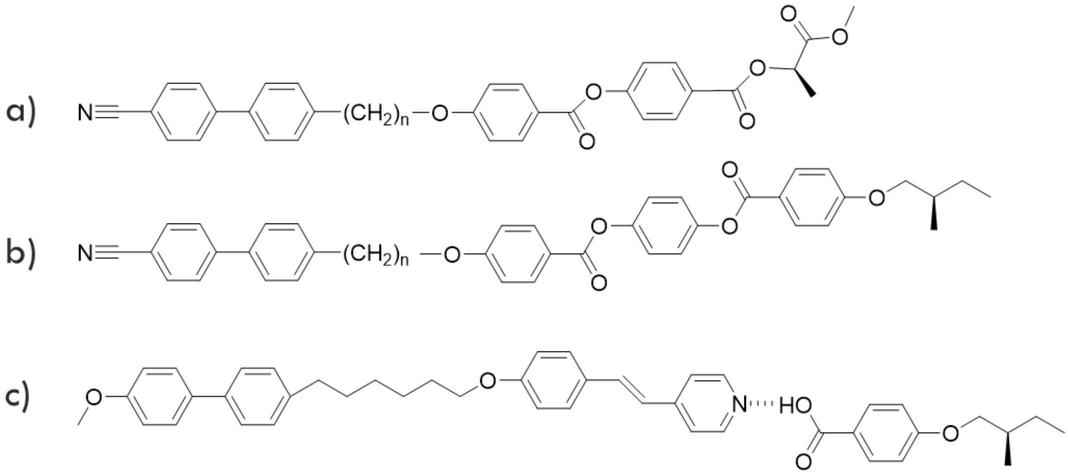

Figure 1. a) *CBnOPEPE(Me)E1, b) CBnOPEPEPO4* and c) 1OB6OS:4*OBA*

In the present work, we summarise a series of projects investigating the properties of the chiral twist-bend nematic phase. Specifically we vary the nature of the chiral centre in a range of new materials designed to exhibit the N^*_{TB} phase: cholesterol-based dimers, the CB*n*OPEPE(Me)E1 series, the CB*n*OPEPEPO4* series (where n = 6, 8, 10), and hydrogen-bonded dimers 1OB6OS:4/*4OBA.

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O27. Hydrogen-bonded liquid crystal tetramers and the twist-bend nematic phase

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Abstract

The recent discovery of the twist-bend nematic phase, N_{TB}, predicted by Meyer [1] and Dozov [2], has caused considerable excitement in the liquid crystal community. In the N_{TB} phase, the director exhibits periodic twist and bend deformations forming a conical helix. The director is tilted with respect to the helical axis and therefore can be considered as a generalised case of the standard chiral nematic phase in which the director is orthogonal with respect to the helical axis. The N_{TB} phase was first discovered experimentally for methylene linked cyanobiphenyl dimers, CBnCB, containing an odd parity spacer to produce a bent structure [3]. Early and extensive research has shown the N_{TB} phase to be critically dependent on the molecular curvature.

In searching for new twist-bend nematogens, the first example of a compound in which the N_{TB} phase is stabilised by hydrogen bonding, namely 4-[6-(4’-cyanobiphenyl-4-yl)hexyloxy]benzoic acid, CB6OBA, has been reported. The phase behaviour shown by CB6OBA is accounted for by the formation of a supramolecular trimer in which the central mesogenic unit is assembled by hydrogen bonding between two benzoic acid units [4].

In this work, the first supramolecular tetramers stabilized by hydrogen bonding to exhibit the twist-bend nematic phase have been investigated. These tetramers are formed by mixing a benzoic acid moiety, namely 4-(8-[4-(4’-cyanobiphenyl)octyloxy]benzoic acid, CB8OBA, with different bipyridines with spacer units of n = 0, 3, 5, 7 and 9; namely 4,4’-dipyridyl, 4,4’-trimethylenedipyridine, 4,4’-pentamethylenedipyridine, 4,4’-heptamethylenedipyridine and 4,4’-nonamethylenedipyridine. Mesophases and transition temperatures have been confirmed by Polarised Optical Microscopy and Differential Scanning Calorimetry respectively. Fourier-transform Infrared Spectroscopy has confirmed the presence of hydrogen bonding between the bipyrdine and benzoic acid moieties, and the coexistence of several supramolecular species in a temperature-dependent equilibrium. These species include the heterocomplexes formed between pyridyl and benzoic acid units, but also hydrogen bonded dimers between benzoic acid units as well as chain-like catemer aggregates. The change in this equilibrium across different phases provides an insight into the role of these species in the stabilisation of the N_{TB} phase.

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O28. Effect of molecular chirality on the nanostructure of a twist-bend nematic phase

Antal Jakli[1], Miroslav Salamonczyk[2,3], Matthew Murachver[3], Ahlam Nemati[3], Torsten Hegmann[3], Chenhui Zhu[4], James Gleeson[3], Samuel Sprunt[3], Muhammad Salili[5], Haumed Rahmani[3]

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Abstract

Dimeric molecules connected with flexible spacers of odd-numbered methylene units exhibit a “twist-bend” nematic (TB) phase characterized by a heliconical pitch of the order of 10 nm. [1-3]. The addition of chiral dopants to achiral dimers [4] in the nematic phase lead to a helical structure, where the micrometer range pitch could be tuned by electric [5] or magnetic [6] fields. Previous

textural studies in the N* phase showed undulation instabilities as a result of the anomalously small bend elastic constant of the material. [7]

Here we carried out DSC, Resonant Soft x-ray (RSoXS), polarized optical microscopy (POM and Phi-Viz Imaging System) and Induced Circular Dichroism (ICD) studies in the TB phase of KA(0.2) [1] doped with ZLI811 from 0 to 3%. We find that the chiral dopant-induced micron-scale helix is expelled in the N_{TB}* phase, while the nanoscale pitch increases from 20 nm to 32 nm from 0 to 3wt% chiral dopant. This increase is much stronger than was found in CB7CB mixed with 5CB where 37% 5CB caused only 20% increase [9]. ICD measurements on the chiral doped samples show strong signal in the N* phase, which then gradually decreases in the TB^* phase. The results show the formation of a twist grain boundary TB phase above 1.5% chiral dopant.

Acknowledgement: This work was supported by NSF DMR No. 1307674 and DMR-1506018. The Advanced Light Source is supported by the Director, Office of Science, Office of Basic Energy Sciences, of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.

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O29. Novel phase behaviour in bent-core nematic liquid crystal mixtures

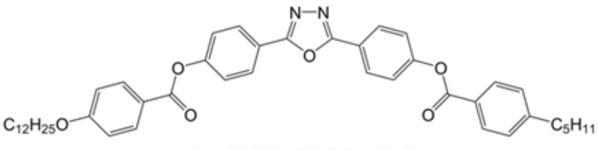
Shajeth Srigengan[1]***, Mamatha Nagaraj***[1]***, Richard Mandle***[2]***, Stephen Cowling***[2]***, John Goodby***[2]***, Helen Gleeson***[1]

[1]University of Leeds, Leeds, United Kingdom. [2]University of York, York, United Kingdom

Abstract

Bent-core nematic liquid crystals (NLCs) are an interesting topic of research due to markedly different behaviour when compared to standard calamitic liquid crystals. The differences include increased flexoelectricity[1,2] and the potential to exhibit exotic phases such as the twist-bend nematic phase[3] and the dark conglomerate phase[4,5].

We investigate the phase behaviour of a series of mixtures of an oxadiazole based bent-core NLCs (compound 1 in Fig. 1) with a number of calamitic liquid crystals respectively. By adding a small percentage (~5-10%) of the bent-core mesogen to the calamitic liquid crystal, a fascinating filament structure is formed[6]. These filaments tend to form when the bulk mixture is in a liquid crystal phase regime but still reside when the sample is heated into the isotropic phase. The filaments can be “melted” by heating the sample to higher temperatures and form again when the sample is cooled back into a liquid crystal phase. This melting and forming of the filaments is reversible. We investigate the nature of the filaments, how they form in the bulk mixture and their stabilisation properties.



Iso 230 N 170 DC 100 Cr

Fig. 1 Molecular structure and phase transitions for compound 1 where the transition temperatures are recorded in °C, and Iso=isotropic phase, N=nematic phase, DC=dark conglomerate phase and Cr=crystalline phase.

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The author would like to acknowledge the EPSRC and MERCK for funding

O30. The twist bend nematic phase in biphenyl-ethane based copolyethers

Warren Stevenson[1]***, Jianggen An***[2]***, Xiang-bing Zeng***[1]***, Min Xue***[2]***, Heng-xing Zou***[2]***, Yong-song Liu***[2]***, Goran Ungar***[1,2]

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Abstract

For several years the transition between the conventional nematic (N) and twist bend nematic (N_{tb}) phases has been a highly topical subject of research. The novelty of the latter phase lies in its unique helical structure, wherein achiral bent molecules tilt at an angle to the pitch axis, but lack long range positional order.[1-3] The transition has been investigated in a wide variety of liquid crystal samples, but so far only one polymeric sample type is known to exhibit the N_{tb} phase: odd spacer copolyethers, featuring flexible biphenyl-ethane mesogens.[4-6]

In light of recent findings, particularly in bent liquid crystal (LC) dimers, we have performed an up-to-date characterisation of the N_{tb}-N transition in the main chain copolythers.[7] Grazing incidence X-ray scattering revealed the N_{tb} phase could be highly aligned by shearing, more so than in LC dimers. This was evidenced by a four-point wide angle X-ray scattering pattern, which originates from convolution of two tilt distributions. Through intensity simulation the orientational order parameter associated with each of the distributions, as well as the conical angle of the N_{tb} phase, were calculated. Information regarding the polymer chain conformation was obtained using polarised IR spectroscopy. The findings suggest the average conformation of the chains is also helical and that the bend angle between mesogenic units decreases with increasing temperature. All experimental evidence, including a jump in birefringence at the N_{tb}-N phase transition, shows that the copolyethers mirror the behaviour of bent LC dimers in almost every respect. This confirms the N_{tb} phase in copolyethers is indeed the same as that in LC dimers.

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O31. Solution of the puzzle of smectic-Q: The phase structure and the origin of spontaneous chirality

***Huanjun Lu*[1]*, Xiangbing Zeng*[1]*, Goran Ungar*[1,2]*, Christian Dressel*[3]*, Carsten Tschierske*[3]**

[1]University of Sheffield, Sheffield, United Kingdom. [2]Zhejiang Sci-Tech University, Hangzhou, China. [3]Martin-Luther University Halle-Wittenberg, Halle, Germany

Abstract

The so-called Smectic-Q phase (SmQ) liquid crystal phase has been discovered in 1983 in rod-like molecules, but its structure remain unclear in spite of numerous attempts to solve it.

Here we present what we believe to be the solution: a unique bicontinuous phase that is non-cubic and is made up of orthogonal twisted columns with planar 4-way junctions.[5] While previously SmQ had only been seen in chiral compounds, this chiral phase has also been found to form also in achiral materials through spontaneous symmetry breaking. The results strongly support the idea of helical substructure of bicontinuous phases and long-range homochirality being sustained by helicity-matching at network junctions. The model also explains the triangular shape of double-gyroid domains growing within a SmQ environment. SmQ-forming materials hold potential for applications such as circularly polarized light emitters, requiring no alignment or asymmetric synthesis.

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O32. The ox-phos wars - and the properties of the inner mitochondrial membrane

John Lydon

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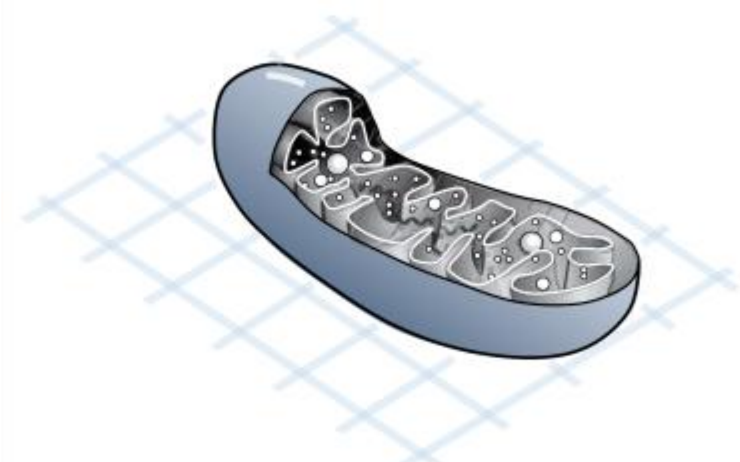
Abstract



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Are you serious, Dr Mitchell?

One of the best stories in the history of biochemistry concerns the pitched battle which lasted for two decades between the 1960s and 1980s. It concerned the mechanism by which cells produce ATP by oxidative phosphorylation. It was an unbalanced conflict. Virtually the whole of the international biochemical establishment was aligned on one side, and on the other was one eccentric British biochemist called Peter Mitchell. His suggestion that the immediate energy source was a proton gradient across the inner mitochondrial membrane [1] was widely scorned as fanciful and unnecessary. Sir Hans Krebs spoke for the majority when he asserted that – “the ‘bag of enzymes concept’ is an adequate description of the cell and there is no need to propose mysterious new forces”.

Mitchell’s Chemi-osmotic theory, has subsequently been described as “the single most counterintuitive idea in biology after Darwin, and the only one to bear comparison with the concepts of Heisenberg, Schrödinger, and Einstein” [2]. It hangs on the remarkable collection of properties inherent in the liquid crystalline state of the phospholipid bilayer. This is far more than a passive barrier dividing the cell into a number of reaction vessels. It is the universal substrate for all life.

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Poster Presentations

P1. B7 liquid crystal filament growth in the presence of carbon nanotubes

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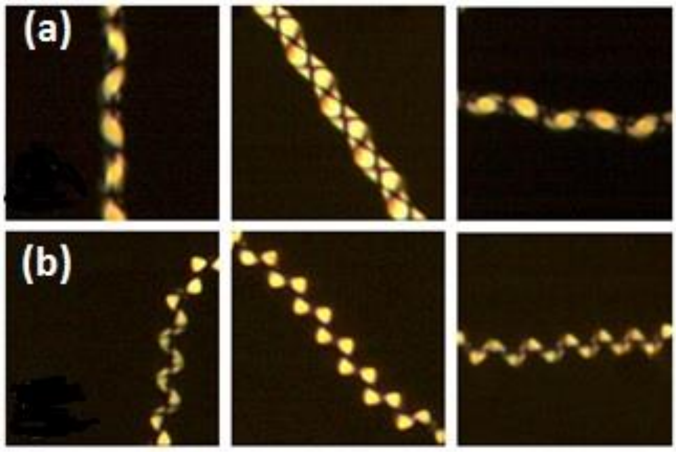
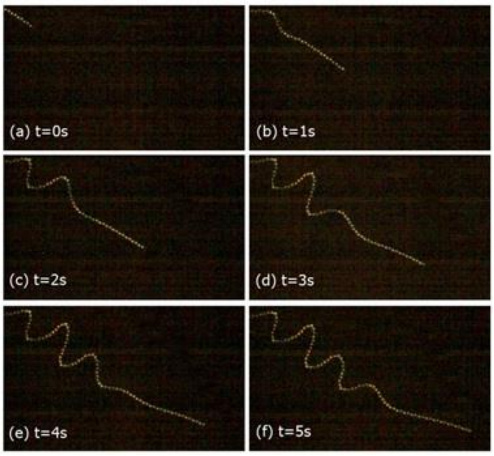
Abstract

For the last two decades, liquid crystal phases formed from bent-core mesogens have attracted the interest of the liquid crystal research community. The main reason is the manifestation of chirality effects from achiral molecules, which is caused by steric interactions. One of the most elusive of the bent-core phases is the B7 phase, which at its early stage often forms in a helical filament fashion when cooled from the isotropic melt (left figure). The present investigation is concerned with the growth of such filaments when subjected to an increasing amount of seeds in the form of single walled nanotubes. The principle question was, what are the effects of dispersed nanotubes, which are most often chiral by themselves, on the growth dynamics and helicity of B7 helical filaments. It is found that the filament width slightly decreases in comparison to the neat B7 material, suggesting a more tightly bound structure around the nanotubes, with the nanotubes presumably acting as the core of the helical filament. At the same time, the pitch or periodicity of the helical superstructure is independent of nanotube concentration. The filament growth velocity quickly decreases as nanotubes are added to the B7 phase, for both single and double twisted filaments, indicating that a more tightly bound structure needs a longer time of formation. At the same time, an elastic buckling instability is observed for freely growing filaments in the isotropic melt (right figure).





Left: (a) double and (b) single twisted filaments at orientations of 0^o, 45^o and 90^o with respect to the crossed polarizers.

Right: Time development of an elastic buckling instability for a filament which is fixed at its starting point of growth at another filament.

P2. A lipid-coated liquid crystal droplet biosensor for antimicrobial peptides detection

***Peng Bao**[1]**, Daniel A Paterson**[1]**, George R Heath**[1]**, Patrick L Harrison**[2]**, Keith Miller**[2]**, J Cliff Jones**[1]**, Sally Peyman**[1]**, Jonathan Sandoe**[3]**, Richard J Bushby**[1]**, Stephen D Evans**[1]**, Helen F Gleeson**[1]*

[1]School of Physics and Astronomy, University of Leeds, Leeds, United Kingdom. [2]Sheffield Hallam University, Sheffield, United Kingdom. [3]Leeds Institute of Biomedical & Clinical Science, Leeds, United Kingdom

Abstract

In the past few years, liquid crystal (LC) materials have gained significant attention due to their potential as low cost biosensors. The interaction between biological amphiphiles and liquid crystal molecules at the liquid crystal/aqueous interface can affect the ordering of LC molecule in the bulk. Biosensors based on LC materials, in planar film and droplet forms, have been successfully demonstrated for the detection of various biomolecules, such as proteins, lipids and toxins [1-4].

Here we demonstrate a novel biosensor based on phospholipid-coated nematic LC droplets for the detection of the antimicrobial peptide (AMP) – SMP43, from the venom of North African scorpion Scorpio maurus palmatus [5]. Mono-disperse lipid-coated LC droplets (of diameter 16.7mm ± 1.1%) were generated using PDMS microfluidic devices with flow focusing configuration (figure 1.a). A lipid monolayer was spontaneously coated onto the surface of LC droplets when they were formed in a liposome solution (lipid concentration ~ few mg/ml). This lipid monolayer was the target for AMPs. The disruption of the lipid monolayer by AMPs was detected at relatively low concentrations (~ few uM), indicated by the change of appearance of the droplets, from a typical radial configuration to a “multi-domain” configuration, easily visible by polarizing microscopy (figure 1.c and d).

Compared to previously reported LC droplet biosensors, the LC droplet biosensor with a lipid coating is more biologically relevant – easy to use to detect membrane-related biological processes and interactions. This LC-droplet biosensor could be further developed for wide applications in reliable, low-cost and disposable point of care diagnostics with good sensitivity.

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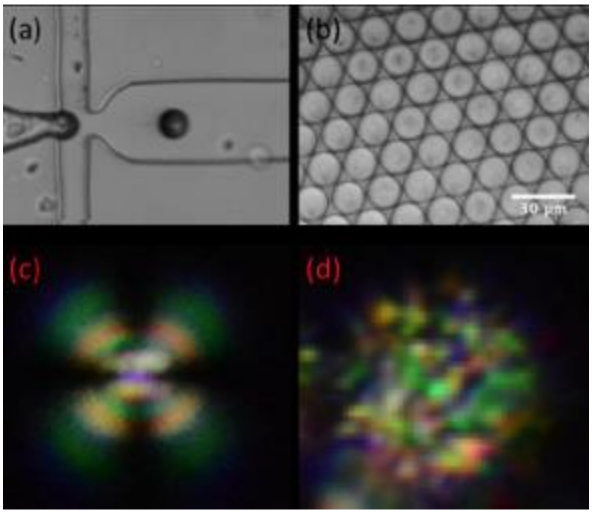

Figure 1 (a) image shows the LC droplet formation in a PDMS device; (b) white light image of the monodisperse LC droplet array; (c - d) the images of the LC droplets under crossed polarizer before (c) and after (d) the exposure to SMP peptides.

P3. Accurate modelling of the optics of high resolution liquid crystal devices including diffractive effects

***Mengyang Yang*[1]*, Zijun Nie*[2]*, Sally Day*[1]*, Aníbal Fernández*[1]**

[1]University College London, London, United Kingdom. [2]University College London, LONDON, United Kingdom

Abstract

The optical behaviour of high-resolution liquid crystal (LC) devices or devices containing small features or LC defects cannot be modelled accurately with the simple methods normally used for traditional display configurations. In this work, an accurate modelling of the liquid crystal structure that yields the order tensor distribution over the complete structure [1,2] is combined with the electromagnetic modelling of waves propagating through the device, calculated using the finite difference frequency domain (FDFD) method.

One of the main difficulties with such an approach is that the numerical solution of the Helmholtz equation involves the solution of large and sparse matrix problems where the matrices are complex, indefinite and frequently, non-symmetric, particularly when absorbing boundary conditions such as the perfectly matched layers (PMLs) are used. The resultant global matrix is normally severely ill conditioned and this makes the most common iterative methods highly inefficient without adequate preconditioning [3]. In this work, a sweeping preconditioner [4] is constructed, specially adapted for this type of problems. The sweeping preconditioner takes advantage of a frontal numbering scheme that correspond to physical layers of the structure. An approximate solution can then be constructed by dividing the structure into subdomains of a few layers and successively finding the approximate solution for these subdomains when the rest of the structure is replaced by PML layers. The resultant preconditioner is then an incomplete block LDU factorization. This approach, to construct a sweeping preconditioner by moving PMLs is particularly appropriate for cases where propagation is mainly one-directional but will not be accurate in cases where there are large reflections or resonances. However, by applying the total-field/scattered-field formulation [5] to construct the matrix problem, this restriction is eliminated making this method effective for all types of problems. The resultant preconditioned matrix problem is then solved efficiently using an iterative technique such as GMRes.

The method will be demonstrated with modelling results for an LC microlens, an LC-based ring resonator and other examples of LC cells containing defects.

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P4. Anomalously low twist and bend elastic constants in an oxadiazole-based bent-core nematic liquid crystal and its mixtures: Contributions of spontaneous chirality and polarity

***<u>Shajeth Srigengan</u>*[1]*, Mamatha Nagaraj*[1]*, Alberta Ferrarini*[2]*, Richard Mandle*[3]*, Stephen Cowling*[3]*, Mikhail Osipov*[4,5]*, Grzegorz Pająk*[6]*, John Goodby*[3]*, Helen Gleeson*[1]**

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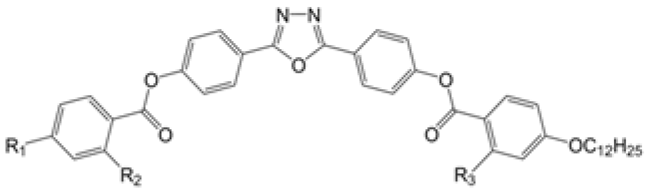
Abstract

Bent-core nematic liquid crystals (NLCs) are an interesting topic of research due to markedly different behaviour when compared to standard calamitic liquid crystals. The differences include increased flexoelectricity[1,2] and the potential to exhibit exotic phases such as the twist-bend nematic (N_{TB}) phase[3] and the dark conglomerate (DC) phase[4,5].

We investigate the phase behaviour of a series of mixtures of two oxadiazole based bent-core NLCs (compound 1 and 2 in Fig. 1), exploring the role the elastic constants play[6]. Knowing that the elastic constants play a part in the formation of the N_{TB} phase, examining how they affect the formation and stabilisation of the DC phase in these mixtures would allow a deeper understanding of these systems.



Compound 1: $R_1 = C_5H_{11}$, $R_2 = R_3 = H$ Iso 230 N 170 DC 100 Cr
Compound 2: $R_1 = C_{12}H_{25}O$, $R_2 = Me$, $R_3 = Ome$ Iso 115 N 88 SmX 64 Cr

Fig. 1 Molecular structure and phase transitions for compounds 1 and 2 where the transition temperatures are recorded in °C, and Iso=isotropic phase, N=nematic phase, SmX=smectic phase of unknown type, DC=dark conglomerate phase and Cr=crystalline phase.

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P5. Design of tunable microwave filters based on liquid crystal

***Ming Lei*, Anibal Fernandez, Clive Poole, Sally Day**

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Abstract

Liquid crystals are a promising material to use in microwave applications due to their tunability and low loss at microwave frequencies [1], [2]. LCs can be tuned by a low voltage and have the advantages of low cost and relative ease of fabrication for different designs. A flexible method to design a tunable microstrip bandpass filter using LC is presented.

A structure has been chosen to demonstrate the design process, based on the filter structure from [3]. There are three stages to the process, two using standard simulation software and the final stage is fabrication and testing. The first stage uses a lumped component simulation using ADS [4], where the structure is approximated to capacitor and inductor elements. This gives the S-parameters and frequency response and allows the first stage of optimisation. Then the 3D EM simulation is carried out with CST Microwave studio 2017 [5]. In this process, the LCs are defined as anisotropic materials, and the alignment directions of LC is approximated as a uniaxial material between substrates. In this way the un-switched and switched states can be modelled. CST allow visualisation of the E field of the microwaves, which allows an estimate of the quality of the simulation since is it known where the LC switching is likely to be non-uniform. Next the dimensions of the filter are optimized to give the largest tuning range. The final stage is the fabrication process and testing. For this paper the micro-strip structures were made using etched Rogers Duroid 5880 substrates; the bottom layer and spacers were made by laser cutting. PVA made by Sigma-Aldrich was used as the alignment layer and E7 LC was used. The measurement setup consisted of a network analyser supplying and measuring the microwave signal to the LC filter. A bias-T connector was used to decouple the bias voltage source from the analyser. The bias voltage was required to switch the liquid crystal.

A good agreement was found between the CST simulation and the measured results from the fabricated device. The small discrepancy in the switched state can be investigated further using a finite element modelling to see the detailed switching of LCs, particularly the narrow layer next to the alignment which remains un-switched.

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6.

P6. Dissipative particle dynamics simulations of worm-like micelles

***Charlie Wand*, Paola Carbone, Andrew Masters**

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Abstract

Worm-like micelles (WLM) are long, self-assembled structures formed by surfactants at high concentrations. Due to the threadlike structure these micelles share many features in common with polymeric systems with an additional relaxation process of micelle breaking/forming. Thus, they are often thought of as ‘living’ polymers. These WLM systems demonstrate complex rheological behaviour that is heavily dependent on many factors, including the surfactant composition and temperature. In addition, the salt

concentration is particularly important for ionic surfactants that are common in industrial applications, such as oil recovery, detergents and personal care products.

There is a well-established theory developed by Cates and co-workers [1] that relates the microscale structure to the macroscopic properties of these complex fluids. One key parameter is the scission free energy, that is, the change in free energy upon breaking a cylindrical micelle into two hemispherical caps (see Figure 1). This can be directly related to the mean micelle length and mean aggregation number.

Here we use Dissipative Particle Dynamics simulations (DPD) to calculate the scission free energy. We employ a simulation protocol developed by Wang *et al* [2]. Briefly, we simulate an infinitely long micelle composed of SLES and CAPB surfactants and calculate the scission free energy using umbrella sampling and the weighted histogram analysis method (WHAM). The reaction coordinate chosen is the number of tail beads in a denoted scission region which has been shown to give a robust calculation of the scission free energy. From these simulations, we are investigating the how the DPD model employed and salt concentration affect the scission free energy.

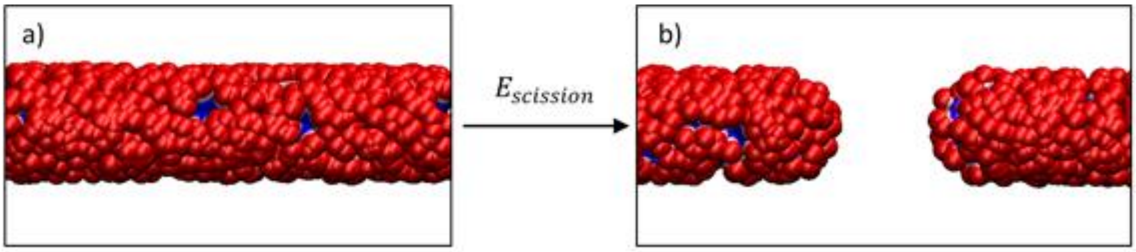

Figure 1 The scission free energy is the change in energy from breaking a wormlike micelle (a) into two hemispherical caps (b).

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P7. Exploring the impact of achiral bent-core molecules as dopants in a chiral nematic phase

***Martin Walker**, Gary Yu, Mark Wilson*

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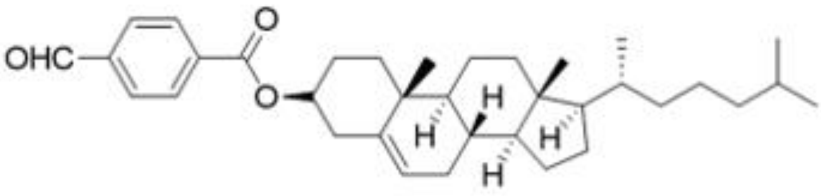
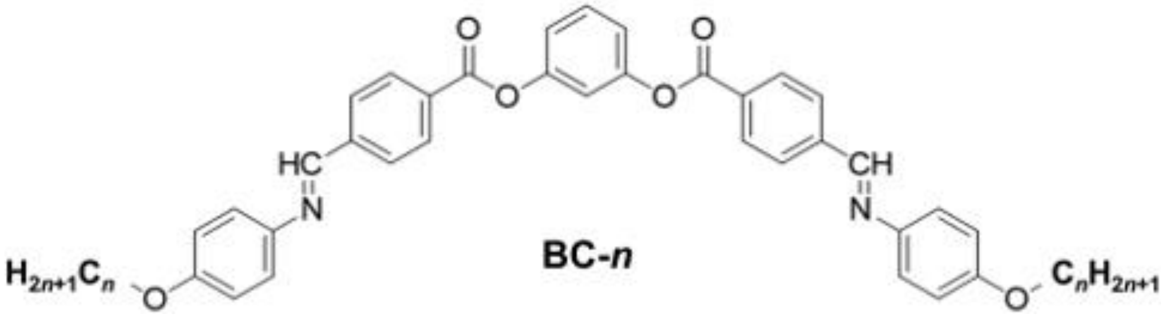
Abstract

Adding chiral dopants to a nematic phase produces the well-known chiral nematic (cholesteric) phase (N*). Conversely, adding achiral dopants to an N* phase dilutes the chirality and therefore increases the pitch length. However, when achiral bent-core molecules, such as 1,4-phenylene bis[4-(4-*n*-alkoxyphenyliminomethyl)benzoates (BC-n below), are added to the N* phase of cholesteryl 4-formylbenzoate, the pitch length decreases.[1] Moreover, remarkably, the decreasing pitch length can be enhanced by increasing the length of the flexible-terminal-achiral-aliphatic chain.[2] This unexpected outcome is in direct conflict with the "established knowledge" of the behaviour of dopants in chiral phases.



Ch compound



BC-*n*

We use atomistic simulation to calculate the helical twisting power (HTP)[3,4] of a range of bent-core molecules in a thermodynamically accessible ensemble of configurations. The resulting distribution of HPT values shows that all the molecules studied have a symmetric distribution centred around zero (m^{-1}), as expected for achiral molecules. However, transient configurations can have exceptionally large HTPs, up to 2 orders of magnitude larger than the best commercial chiral dopants. We hypothesise that intermolecular interactions between transient conformations, which have exceptionally high HTP values, leads to symmetry breaking and preferential selection of enantiomeric conformers that induce a helical twist in the same direction as the host phase. Simulations to demonstrate this conformational selectivity are underway in our laboratory.

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P8. Inexpensive, operationally simple flow reactor for rapid, chromatography free synthesis of siloxane based liquid crystals

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Abstract

Siloxanes are commonly employed as a terminal group in liquid crystals due to their tendency to reduce melting points and stabilise smectic phases. The synthesis of these materials is typically performed using homogenous late transition metal catalysts which are expensive, non-recoverable and can contaminate the resulting product with trace metal impurities. We have devised an inexpensive (<£300) flow reactor constructed out of standard modular laboratory hardware and using a 'Karstedt-like' catalyst on silica gel (Pt @ SiO_2) as a catalyst bed for the production of liquid crystalline siloxanes in a continuous process. [1] Conversions are quantitative, and the entire process is chromatography free; at the end of the run the solvent is removed *in vacuo* to leave the analytically pure material. We have used this technique to synthesise a family of cyanobiphenyls bearing siloxanes as terminal groups, and we contrast their properties to literature examples.

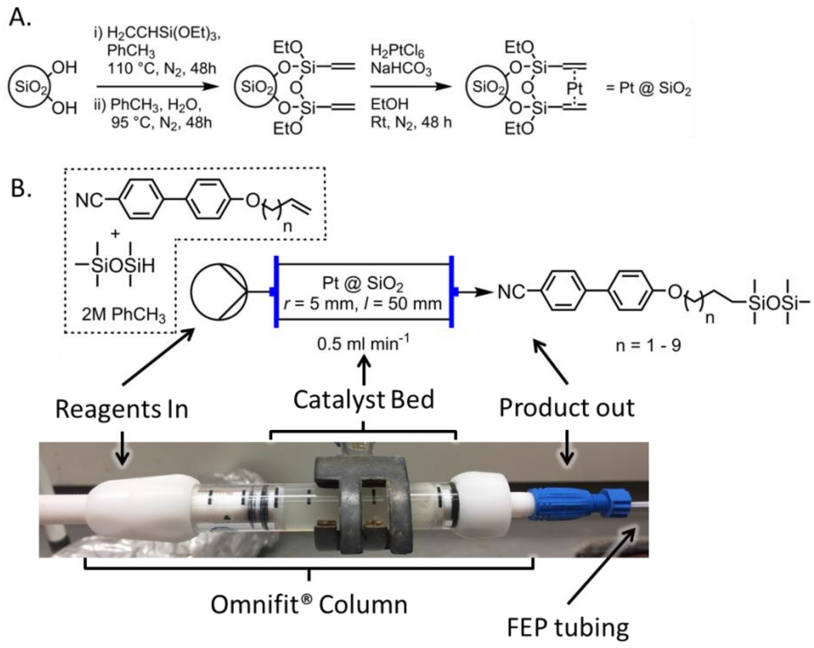

Figure 1: (a) synthesis of Pt @ SiO_2, (B) continuous flow production of siloxane terminated cyanobiphenyls.

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P9. Janus dendritic liquid crystals

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Abstract

Dendritic liquid crystals show a rich self-assembling behaviour that is exquisitely modulated by the molecular parameters of each of the many components of the supermolecule [1-3]. The nature of the mesogens incorporated as end groups, nature of the core, type and multiplicity of the dendritic branches and spacer lengths at each of these elements are key design elements that influence the mesophase behaviour. In this context we have reported Janus dendritic liquid crystals, those featuring two different dendritic lobes attached to a central *flexible scaffold* (A, B, Figure 1)[1]. In addition, mutually incompatible groups such as hydrocarbon and fluorocarbon offer further opportunity to realise complex mesophase morphologies when they are present in the same molecule in a segregated fashion [4].

Following from our work on supermolecular liquid crystals, in this report we describe a family of Janus dendritic liquid crystals featuring a central *rigid scaffold* (Figure 1). These materials have been designed to feature fluorocarbon, hydrocarbon, and cyanobiphenyl mesogenic units in varying ratios to investigate the interplay of molecular curvature and nanophase segregation. Their mesomorphic behaviour depends on the nature and relative number of substituents placed at the dendritic lobes at either side of the core, and their ability to induce nanophase segregation.

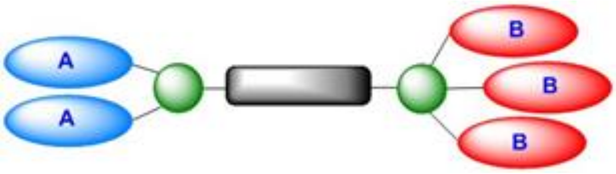

Figure 1. Schematic representation of Janus dendritic liquid crystals.

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P10. Liquid crystal dimers and the twist-bend nematic phase

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Abstract

The most recently discovered liquid crystal phase, the twist-bend nematic, N_{TB}, is fascinating for a multitude of reasons but in particular for, the observation of spontaneous symmetry breaking in a system composed of achiral molecules. First predicted by Meyer [1] and later independently by Dozov [2], the directors in the N_{TB} phase form a helix, and are tilted with respect to the helical axis. The induced twist may be either left- or right-handed and equal amounts of both types of helix are expected. Experimentally, the N_{TB} phase was unambiguously observed by Cestari *et al* [3] in CB7CB, a symmetrical dimer consisting of a heptamethylene spacer linking two cyanobiphenyl mesogenic units. In designing new twist-bend nematogens, the key structural feature appears to be molecular curvature[4]. Apart from odd-membered dimers, the N_{TB} phase has been also observed in bent-core materials [5], and hydrogen bonded dimers [6] and conventional trimers.

Here we describe the synthesis and characterisation of a range of new non-symmetric liquid crystal dimers designed to exhibit the N_{TB} phase, see Figure 1. These comprise of either a cyano or methoxy biphenyl unit, linked by an alkoxy spacer to a benzoic acid moiety. Additionally, we report how the introduction of a benzamide or benzamine moiety impacts mesogenic behavior. Furthermore, through esterification with the large aromatic bent-core shon in figure 1(b) [7] will investigate the impact of increased molecular curvature on phase behaviour.

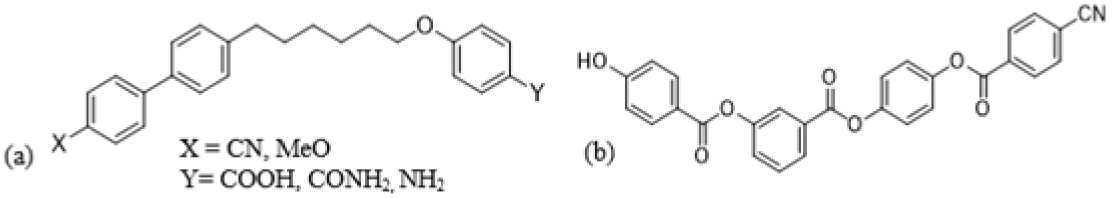

Figure 1: (a) General structure of calamitic dimer, (b) Aromatic bent core used in the making of Banana-calamitic dimers.

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P11. Liquid crystal trimers exhibiting twist-bend nematic behaviour

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Abstract

The twist-bend nematic phase, N_{TB}, is the most recently discovered nematic phase. It was first predicted by Meyer [1], then later independently by Dozov [2]. The N_{TB} phase is observed for molecules having an overall bent structure. These bent molecules tend to ‘nest’ within each other to form groups of molecules with an overall bent shape. To fill space, the directors form a helix and are tilted at an angle Ɵ relative to the helical axis.

The overwhelming majority of twist-bend nematogens are liquid crystal dimers consisting of molecules containing two mesogenic units linked through a flexible spacer. If an odd-number of atoms connect the two mesogenic units then the prerequisite bent-shape is achieved. The most studied liquid crystal dimers exhibiting the twist-bend nematic phase belong to the CBnCB series [3-4], in which two cyanobiphenyl units are linked by an alkyl spacer. Recently higher oligomers, both covalent and hydrogen bonded and containing various mesogenic units have also been shown to exhibit the N_{TB} phase. [5-7]

Here we report the synthesis and characterisation of novel liquid crystal trimers based on biphenyl or benzylideneaniline liquid crystal groups. To maintain an overall bent structure the flexible spacers between the aromatic mesogens are of odd parity.

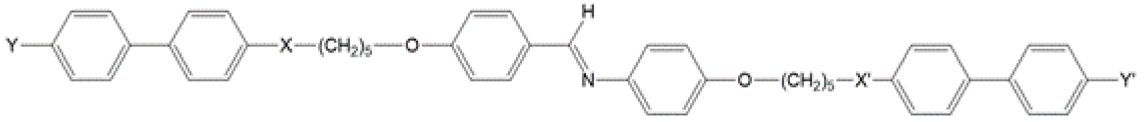

Figure 1: Structural skeleton of synthesised liquid crystal trimers containing biphenyl or benzlideneanaline mesogenic units. (Y, Y’ = CN or OMe; X, X’ = CH_2 or CO)

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P12. Molecular dynamics simulation of a smectic-A: do the viscosities diverge?

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We present molecular dynamics results on the transport coefficients of a smectic-A liquid crystal. These properties are of particular interest due to theoretical claims that four of the five smectic-A viscosities are divergent at zero frequency, diverging as the inverse of the frequency [1]. This divergence is predicted to occur via the coupling of elements of the stress tensor to layer fluctuations. There is some limited experimental evidence in support of this divergence, but it is of insufficient sensitivity to quantitatively test theory [2-5]. Computer simulations can hopefully cast further light on this phenomenon.

We study a system of 9000 Gay–Berne particles. Details of the model are given in [6]. Our simulations reveal anomalous single particle rotational diffusion, similar to that previously observed in a nematic [6], but our main result is that the stress–stress autocorrelation functions appear to show no significant long time behaviour. This translates into normal, non-diverging viscosities at zero frequency, at odds with theoretical predictions. We will present possible reasons for this discrepancy.

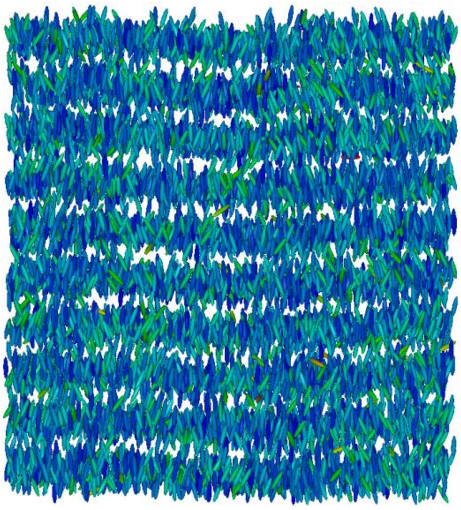

Figure 1. Snapshot of the Smectic-A system.

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P13. Molecular shape as a means to control the incidence of the nanostructured twist bend phase

Emily Pocock, Richard Mandle, John Goodby

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Abstract

We devised a simple synthetic route to Br8CB and used this intermediate to construct a family of unsymmetrical bimesogens analogous to CB8OCB, reported by us previously. [1] Methylene linked dimers exhibit a linear relationship between $T_{NTB\text{-}N}$ and $T_{N\text{-}Iso}$, and we observe a similar relationship (with identical slope) for the mixed methylene/ether linked dimers in this work. The difference in behaviour between methylene- and methylene/ether- linked materials appears to be a product of molecular shape; changes to molecular structure do not affect the relationship between the two transition temperatures. [2]

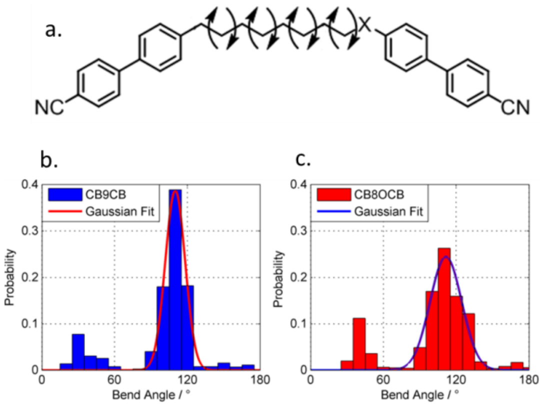

Figure 1: The structure of CB9CB (X = -CH_2-) and CB8OCB (X = -O-). Arrows denote bonds allowed to undergo threefold rotation during the conformational search. Histogram plots showing the probability of a given intermesogen angle for CB9CB (b) and CB8OCB (c) along with Gaussian fits (solid lines) to the major peak centred at ~ 105 °.

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P14. Novel bolaform - modified lipid molecules for liquid crystal droplet formation with bipolar alignment

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Abstract

It has long been known that liquid crystals (LC) respond to external stimuli and can be reconfigured accordingly. Recently however, a series of studies have demonstrated the design of LC materials with possible biological applications [1]. A key challenge in designing LC materials for such applications is in tailoring the interfacial interaction between biological amphiphiles and LC at the liquid crystal/aqueous interface.

It has been shown that typically for lipid coated LC films, a homeotropic alignment is observed, but recent studies into bolaform units have demonstrated the possibility of tailor made bolamphiphile units to align the LC in planar arrangement [2]. In this poster we demonstrate synthesis of novel PC lipids containing bolaform end units and their ability to form lipid bilayers (Figure 2).

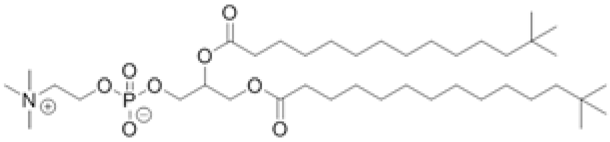

Figure 1. Example of the type of bolaform- modified lipid used in this study

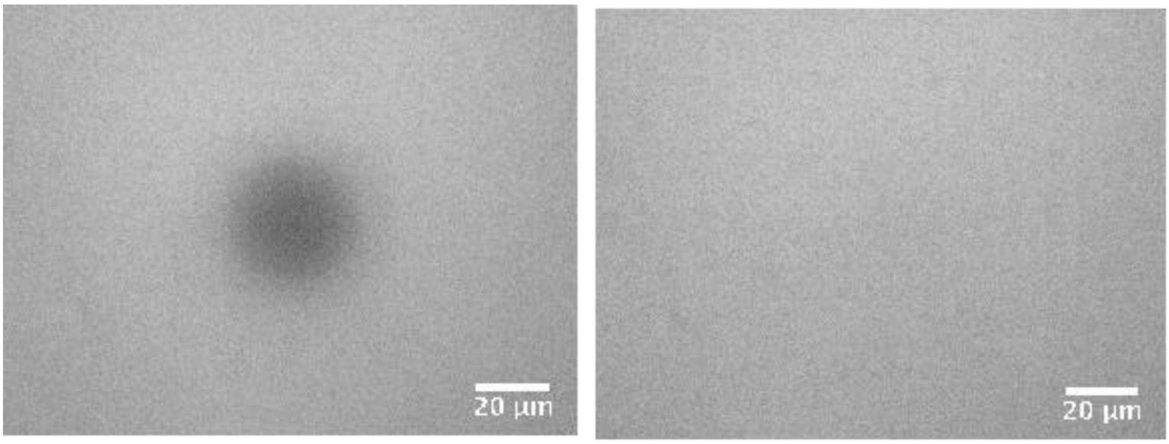

Figure 2. FRAP (Fluorescence recovery after photobleaching) for a supported bilayer of the bolaform – modified lipid on glass. (left: bleached; right, recovered)

LC droplets (MLC2081) coated with a monolayer of bolaform modified lipid have been shown to exhibit the first example of a lipid coated LC droplet with bipolar alignment (Figure 3).

LC droplets with this type of modified alignment have possible use as a more biologically applicable biosensor than previously reported biosensors based on LC materials [3-6].

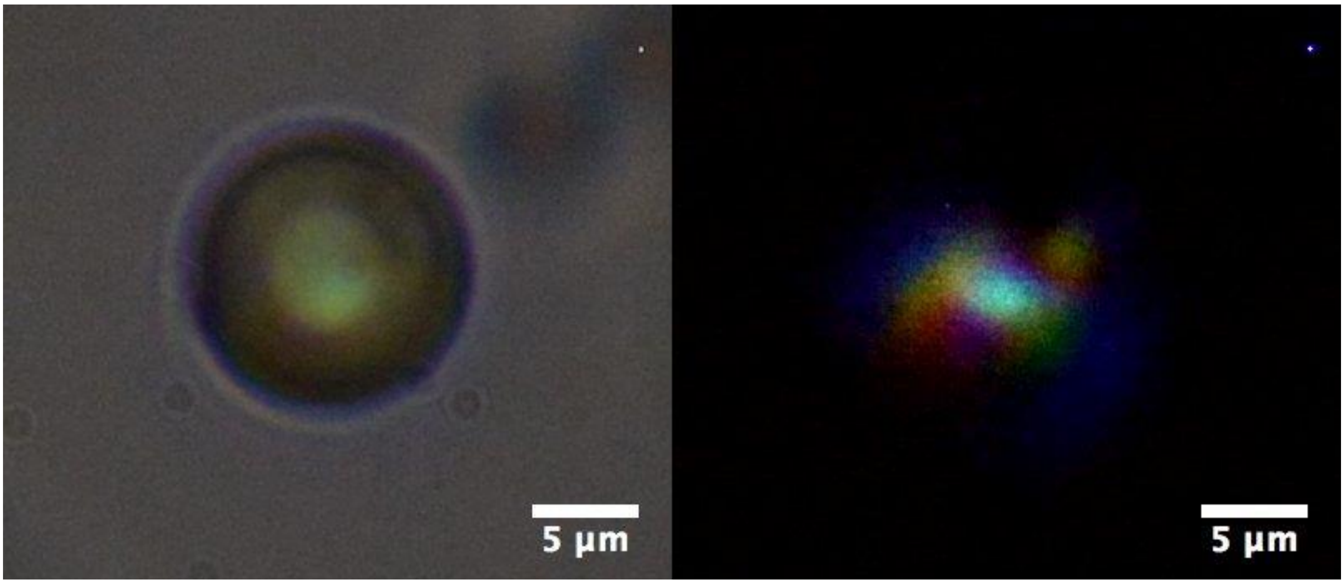

Figure 3. Micrographs of LC droplets in bipolar arrangement in transmission mode and between crossed polarisers.

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P15. Prediction of EPR spectra of lyotropic liquid crystals using a combination of molecular dynamics simulations and the model-free approach

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Abstract

EPR with paramagnetic spin probes combined with molecular modelling have proved to be a particular useful approach for the study of the dynamics and order in thermotropic liquid crystals (e.g. nematic, discotic) [1-3].

We report the first application of fully atomistic molecular dynamics (MD) simulations to the prediction of the motional electron paramagnetic resonance (EPR) spectra of lyotropic liquid crystals in different aggregation states doped with a paramagnetic spin probe [4]. The purpose of this study is twofold. First, given that EPR spectra are highly sensitive to the motions and order of the spin probes doped within lyotropic aggregates, simulation of EPR line shapes from the results of MD modelling provides an ultimate test bed for the force fields currently employed to model such systems. Second, the EPR line shapes are simulated using the motional parameters extracted from MD trajectories using the Model-Free (MF) approach. Thus a combined MD-EPR methodology allowed us to test directly the validity of the application of the MF approach to systems with multi-component molecular motions. All-atom MD simulations using the General AMBER Force Field (GAFF) have been performed on sodium dodecyl sulfate (SDS) and dodecyltrimethylammonium chloride (DTAC) liquid crystals. The resulting MD trajectories were used to predict and interpret the EPR spectra of pre-micellar, micellar, rod and lamellar aggregates. The predicted EPR spectra demonstrate very good agreement with most of experimental line shapes thus confirming the validity of both the force fields employed and the MF approach for the studied systems. At the same time simulation results confirm that GAFF tends to overestimate the packing and the order of the carbonyl chains of the surfactant molecules.

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P16. Square and hexagonal columnar liquid crystals confined in square and triangular pores

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[1]University of Sheffield, sheffield, United Kingdom. [2]Zhejiang Sci-Tech University, Hangzhou, China

Abstract

In our previous study, we found that columnar liquid crystals confined in cylindrical nano pores under planar anchoring prefer to form circular concentric configuration. We suggested that it is the mismatch between the polygonal columnar lattice and the circular pores that prevents axial orientation. Here we further prove this by confining hexagonal and square columnar phases in equilateral triangle and square pores, respectively. X-ray diffraction study reveals that while they all adopt circular concentric configuration in circular pores, axial alignment is indeed achieved for the hexagonal phase of a discotic hexa-peri-hexabenzocoronene in *triangular* pores, and for the square phase of a T-shaped amphiphile in *square* pores. For the third compound, a carbazole dendron with very soft hexagonal columns, a new three-domain configuration is directly observed by AFM in triangular pores. A simple estimation of free energies confirms that it is the distortion of polygonal columnar lattice that prevents axial orientation in circular pores. The model also rationalizes the three-domain arrangement of soft columns.

P17. Surfactant self-assembly: Insights from DPD simulation

Sarah Gray, Martin Walker, Mark R. Wilson

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Abstract

Mesophase formation is critical in the design and processing of many household products, but phase behaviour of complex surfactant-additive mixtures remain challenging to predict.

Dissipative Particle Dynamics is a mesoscale simulation method, with the ability to retain molecular detail while simulating at the level of micrometers and milliseconds;[1] making DPD the ideal method to investigate mesophase behaviour as it rapidly maps out phase diagrams.

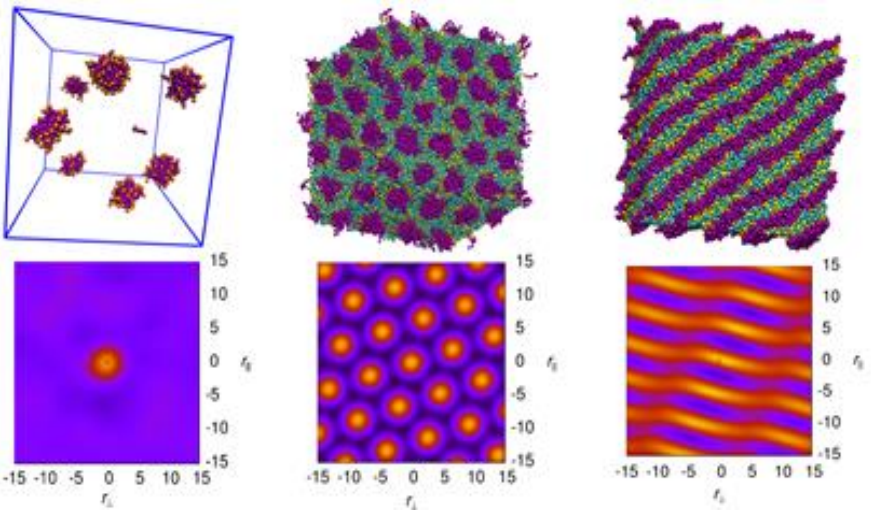

Figure 1 : Typical anionic surfactant mesophases L_1, H_1, and L_α, formed by our model.

We have parameterised a highly transferable DPD model that readily describes phase behaviours of common anionic surfactants (sodium dodecylsulphate, linear alkylbenzene sulphonates, and alkylether sulphonates) across wide concentration ranges and as pure or isomeric mixtures. With this model we have probed how different environments, solvents, additives, and molecular architectures and interactions change surfactant phase behaviour. Our model is a powerful tool in understanding the factors that influence the formation, or breakdown, of ordered phases in surfactant-based mixtures.

Figure 2: Example phases formed by our surfactant models under different geometrical constraints and with changing wall interactions.

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P18. Synthesis and properties of triphenylene dyads

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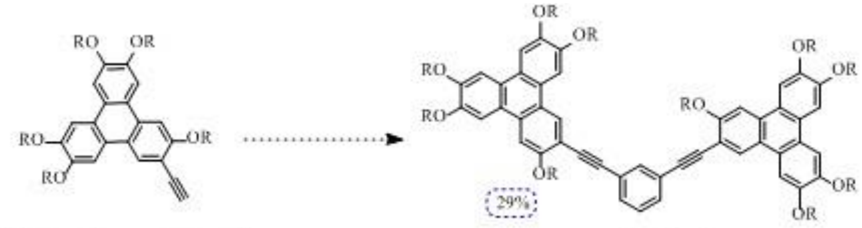
Abstract

Since the discovery of discotic liquid crystals in 1977 by Chandrasekhar[1], this area of research has found significant interest. Triphenylene is one of the most important cores for molecules displaying a discotic mesophase, and has been widely investigated

over the last decade. Previous work in our group has shown that twining triphenylenes through rigid linkers[2] gave rise to nematic mesophase formation rather than the columnar phases which are usually observed[3]. The work described in this poster concerns the successful synthesis of a series of triphenylene dyad derivatives. In the series, two triphenylene units (bearing 5 alkoxy chains) are linked to aromatic cores. The link points (1,2-, 1,3-, 1,4- in benzene and 2,5- in thiophene) determine the overall shape of the dyads. The synthesis of the common intermediate (triphenylene acetylene **1**) is described along with synthesis and mesophase behaviour of the final dyads.



Triphenylene acetylene 1

example of dyad

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P19. The design and investigation of CdSe based nanoparticles linked to nematic mesogens

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Abstract

The design and investigation of CdSe based nanoparticles linked to nematic mesogens

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For nanoparticles (NPs), connected chemically to suitable mesogenic or dendritic groups it has been observed that liquid crystalline (LC) phase behaviour can be formed. Typically the structure of the LC phases detected depends on the size of the NPs, their coverage with organic groups and the size and shape of these organic groups. This allows to some extend for the control of the phase transition temperatures as well as the addressing of the two or three dimensional arrays of the NPs in the LC matrices. Though a range of NP systems have been epxlored, the focus has so far been mainly on gold or silver based LC NP systems. This is due to their excellent assessabilty and chemical stability. Surprisingly, to the best of our knowledge, there have so far been no reports on CdSe NPs which form LC phase behviour, as examples of quantum dots (QDs) linked to calamitic LC groups.

Here we report the results of our investigations of CdSe NPs linked to laterally connected mesogens for which nematic phase behviour as well as 2D and 3D self assembly behaviour has been reported before. [1] The QDs were prepared in a mulitstep step process using a kinetic grwoth method. [2] In a second stept hexyl thiol groups were inotruced in an exchange reaction. Finally, in a further exchange reaction mesogenic groups were linked to the NPs. The chemcial structure of the QD_LC_NPs was characterised by NMR, transmission electron miscroscpy (TEM), UV/vis spectroscpy and thermogravimetric analysis (TGA) studies. The size of the NPs was determined to be ~3.3 nm based on TEM characterisation. We report the results the investigations of the LC prperties based on optical polarizing microscopy (OPM) and differential scanning calorimetry (DSC) as well as of the formation of the superstructure of the NPs using GISAX. The experiemtnal resutls will be correlated to earleir work on conceptually related NP systems.

P20. The effect of replacing biphenyl units with terphenyl units in liquid crystal mesogens.

<u>Grant Strachan</u>, Corrie Imrie, John Storey

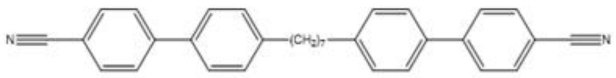
University of Aberdeen, Aberdeen, United Kingdom

Abstract

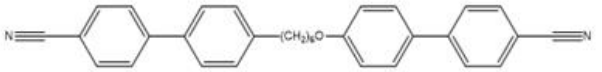
The effect of replacing biphenyl units with terphenyl units in liquid crystal mesogens.

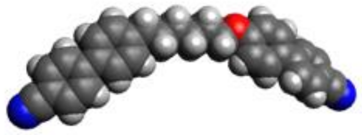
<u>Grant Strachan</u>, Corrie T. Imrie, John M. D. Storey.

The twist-bend nematic (N_{TB}) phase is a liquid crystalline phase in which bent, achiral molecules spontaneously form right-, and left-handed helices. This leads to the formation of domains of opposite handedness within a phase with no net chirality[1,2]. The N_{TB} phase was first discovered for 1,7-bis-4-(4′- cyanobiphenyl) heptane, CB7CB[3]. This molecule consists of two cyanobiphenyl units connected by a flexible aliphatic chain.



The molecular features required to obtain the N_{TB} phase are still under investigation but it is apparent that molecular curvature is required. A closely related molecule to CB7CB, 1-(4-cyanobiphenyl-4′-yloxy)-6-(4-cyanobiphenyl-4′-yl)hexane, CB6OCB, also shows N_{TB} behaviour[4].





The transitional behavior of these two mesogens has been extensively studied, and their general structure of two cyanobiphenyl units linked by a flexible space is archetypal for twist-bend nematogens. There has been a great deal of interest in the effects of varying different sections of this basic structure, such as linking groups, and terminal units[5,6]. Here we report the effect of introducing terphenyl units into the structures to replace one or both biphenyl units.

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P21. Trigonal columnar self-assembly of bent phasmid mesogens

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Abstract

The term ‘‘phasmid’’ mesogen is used to describe rod-likemolecules with three flexible chains, usually alkyl, at each end, and the name refers to the similarity with the six-legged insects known by the same name. Usually such mesogens form the hexagonal columnar (Colhex) liquid crystal (LC) phase, where typically three aromatic rods lie parallel to each other and perpendicular to the column axis, forming a stratum of the column; the alkyls fill the space between the columns. The question is whether a trigonal columnar LC phase can be formed, with three-fold rather than six-fold symmetry and with non-cylindrical columns.

Here we show that columns with a three-arm star cross-section and trigonal symmetry can form from a series of compounds, with a bent rod-like aromatic core and three alkoxy chains at each end, synthesised by click reaction.[1] The columnar liquid crystal phase has a noncentrosymmetric trigonal p31m symmetry. While the crystallographic plane group belongs to the hexagonal system, the phase symmetry is actually trigonal. The finding indicates a potential new path to creating non-centrosymmetric self assemblies that could, with suitable substituents, be used in ferroelectric, pyroelectric or frequency-doubling optical devices.

[1] H. F. Cheng, Y. X. Li, X. B. Zeng, H. F. Gao, X. H Cheng, G. Ungar, Chem. Commun. 2018, **54**, 156-159.