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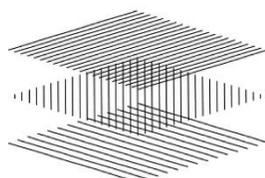
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Faults that are rich are fair: the many beauties of liquid crystal defects

F. Serra^{*a}

^a*Department of Physics, Chemistry and Pharmacy, University of Southern Denmark, Odense, Denmark*

*serra@sdu.dk

Everyone who studies liquid crystals can certainly find many fascinating properties in these materials, but for me nothing is more charming than topological defects. With them, one can study topology with an optical microscope. Moreover, not only can they be used to probe the delicate interplay of topology and energy, but they can also manipulate light, control the motion of colloidal particles, trap molecules and mix active fluids. More and more evidence is building up to show that defects are the tools that nature uses to regulate tissues and generate shapes.

Creating and controlling defects presents challenges, sometimes unexpected. In this talk, I will discuss (some of) the properties and applications of liquid crystal defects, mostly nematic and smectic, and the strategies I have used to manipulate them. After many years, they never cease to surprise: defects end up sliding along colloidal particles [1], making elaborates twists in non-chiral samples [2] or refusing to connect point defects [3].

I will discuss some of these aspects and conclude with an outlook into the future of the field, focusing especially on the recent discoveries of the role of nematic defects in biology.

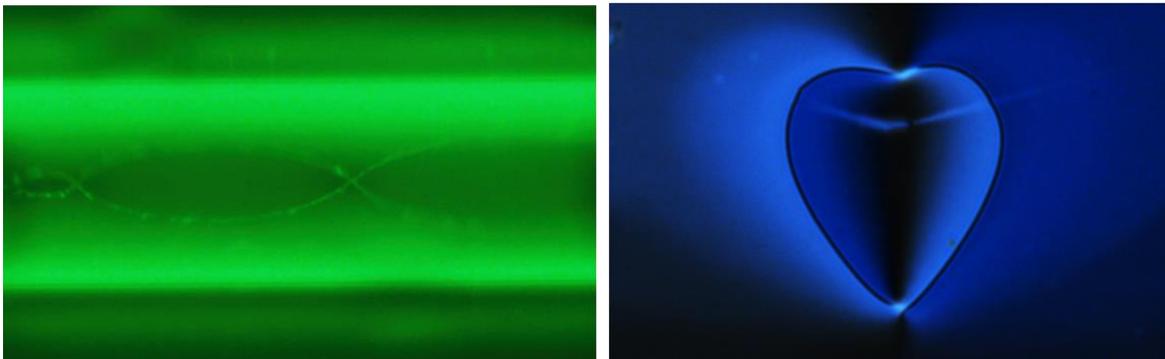


Figure 1. Left: a double helix disclination in a capillary (fluorescence). Right: heart-shaped disclination lines (polarized microscopy).

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The Role of Elastic Anisotropy in Active Nematics

A.J.H. Houston^{*a}, G.P. Alexander^{b,c}

^a Department of Physics, University of York, York, YO10 5DD, UK

^b Department of Physics, University of Warwick, Coventry, CV4 7AL, UK

^c Centre for Complexity Science, University of Warwick, Coventry, CV4 7AL, UK

*alexander.houston@york.ac.uk

The one-elastic-constant approximation has been shown to be especially flawed in active systems due to hydrodynamic instabilities which soften deformation modes, resulting in activity-dependent effective elastic constants [1,2]. This, along with the realisation of a lyotropic nematic with tunable elastic properties [3] has fueled interest in utilising elastic anisotropy as a route to control the behaviour of active nematics. We calculate the active flows around topological defects in active nematics with unequal elastic constants, given in Figure 1, and show that both these and the defect morphology can be understood through the symmetry of the defects themselves. For $+1/2$ defects this reveals a remarkable insensitivity of the active flows of isolated defects to changes in the elastic constants. However, the discrepancy in elastic constants causes defects to exert an orientating torque on each other. This torque both distorts the trajectories of the defects and can be tuned to encourage or inhibit defect pair creation. As a result it has implications for the transition from the ordered to the active turbulent state and may provide a means by which to control the dynamics of active systems.

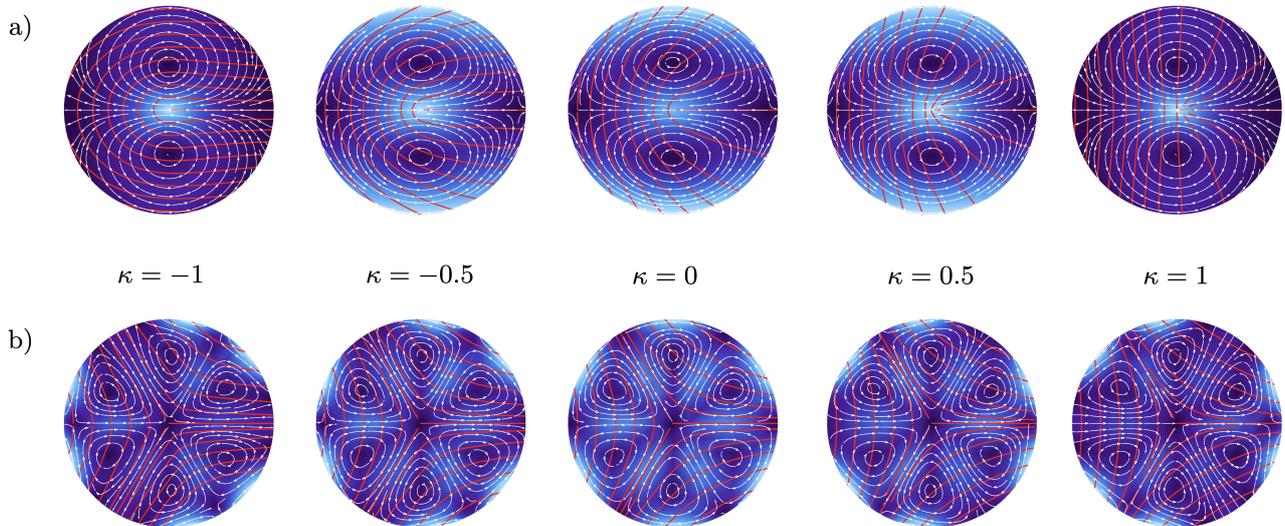


Figure 1: The active flows around a) $+1/2$ and b) $-1/2$ defects as a function of $\kappa = (K_3 - K_1)/(K_1 + K_3)$, with K_1 and K_3 the splay and bend elastic constants respectively. The flow streamlines are shown in white (with arrows), the background colour is lighter when the flow velocity is higher and the red lines indicate the director profile.

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Mathematical modelling of charge effects in liquid crystalline biofilms

Maria van Rossem^{*a}, Sandra Wilks^b, Malgosia Kaczmarek^a and Giampaolo D'Alessandro^c

^a *School of Physics and Astronomy, University of Southampton, Southampton, SO17 1BJ, UK*

^b *School of Health Sciences, University of Southampton, Southampton, SO17 1BJ, UK*

^c *School of Mathematics, University of Southampton, Southampton, SO17 1BJ, UK*

*mtvr1e19@soton.ac.uk

The modelling of charged systems has various applications in soft matter; a recently discovered example is the formation of liquid crystalline biofilms by charged filamentous viruses [1]. These soft matter systems are of strong interest in medicine, since the liquid crystalline structure increases the antibiotic tolerance of the bacteria in the biofilm. *In vivo*, the viruses form tactoids that encapsulate the bacteria: we modelled this system as shown in figure 1 [2]. We found that liquid crystal formation indeed has a strong effect on antibiotic tolerance, mainly through adsorption of the cationic antibiotics by the anionic viruses. We also developed an analytically solvable version of the model using homogenisation, to better analyse the significance of the parameters [3]. In these models, charge effects were modelled implicitly through their effect on antibiotic adsorption.

The importance of adsorption to antibiotic tolerance led us to investigate the charge effects in the system further. We developed a new, extended model which explicitly incorporates the electric field generated by the viruses, antibiotics, and ions present in the solvent. As before, we also derived a homogenised effective equivalent of the model. Our results show that the antibiotic charge greatly impacts the diffusion. Furthermore, we find that the contribution of the antibiotic charge to the screening of the viral surface charge is negligible compared to that of the solvent ions. This rules out the possibility that antibiotics facilitate liquid crystal formation through charge screening. Finally, we derive a correlation between solvent ionicity and virus packing density: this result has been qualitatively confirmed by Secor et al. [1] and we plan to do experiments for quantitative verification.

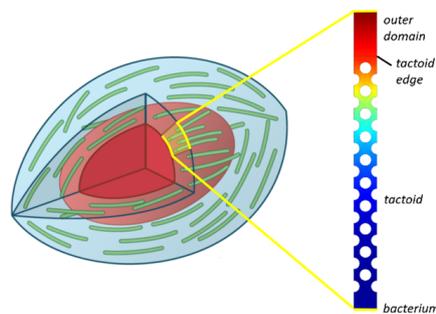


Figure 1: The modelled system: a sketch of a tactoid (in blue) with viruses (green) encapsulating a bacterium (red). A two-dimensional slice of the system (yellow) is taken as the geometry of the mathematical model, as illustrated on the right, with circles representing virus cross-sections and color indicating antibiotic concentration.

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Defects in a Spherical Droplet of Nematic Liquid Crystal

Sophie McLauchlan*^a, Apala Majumdar^a, Yucen Han^a, Matthias Langer^a

^a *Department of Mathematics and Statistics, University of Strathclyde, Glasgow, G1 1XH, UK*

*sophie.mclauchlan@strath.ac.uk

Nematic liquid crystals exhibit key physical properties, intermediate between conventional liquids and solids, with long-range orientational ordering, which make them ideal candidates for a wide array of applications. Confined nematic systems often exhibit complex defect structures due to the competing effects of geometrical frustration and material properties. It is the presence of such defects that gives rise to the striking optical patterns observed in samples of nematic liquid crystals in confinement.

We model configurations of nematic liquid crystals in a spherical droplet with rotational and mirror symmetry constraints within the Landau–de Gennes theory [1]. In particular, we revisit the radial hedgehog solution [2, 3], a canonical degree +1 defect found in a variety of materials such as superconductors and cavitation in elasticity. In the absence of surface energies and external fields, the Landau–de Gennes energy comprises a bulk energy potential, capturing the preferred phase of the nematic liquid crystal; and an elastic energy potential, penalising spatial inhomogeneities. The simplest and most widely used bulk energy potential is the fourth-order bulk potential. We first describe the character of the radial hedgehog solution with the fourth-order potential versus the more complicated sixth-order bulk potential as reported in [4]. We then use a Finite Element Method to find minimisers of the Landau–de Gennes energy with the fourth- and sixth-order bulk potentials for a variety of temperatures and droplet radii. We compute the Morse index of the radial hedgehog solution for a range of temperatures and radii with the fourth- and sixth-order potentials to demonstrate that both models predict the instability of the radial hedgehog at low temperatures and large droplet radii, while the sixth-order potential appears to have a destabilising effect on the radial hedgehog configuration. Moreover, we demonstrate how the Landau–de Gennes free energy with sixth-order potential appears to admit hedgehog configurations with negative scalar order parameter in contrast to the model with the fourth-order potential. We also provide examples suggesting that when the radial hedgehog is an index-1 saddle point, it acts as a transition state between index-0 split core and biaxial torus configurations.

We conclude with a discussion on potential applications of droplets of nematic liquid crystals, which provides context and motivation for this work.

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Defect conformations in 3D active nematics

L. Head^a, R. Keogh^a, L. Angheluta-Bauer^b, J. Viñals^c, **T.N. Shendruk**^{*a}

^a *School of Physics and Astronomy, University of Edinburgh, Edinburgh EH9 3FD, UK*

^b *The Njord Centre, Department of Physics, University of Oslo, Oslo 0316, Norway*

^c *School of Physics and Astronomy, University of Minnesota, Minneapolis, MN 55455, USA*

*t.shendruk@ed.ac.uk

Active nematics are driven out-of-equilibrium by the intrinsic conversion of biochemical energy into mechanical work at microscopic scales. Increasing activity destabilises global nematic order through nematic distortions and induced spontaneous flows sustained by the continuous creation and annihilation of nematic defects. This regime leads to chaotic flows (active turbulence) in the bulk and complex spatiotemporal patterns of nematic defects and their associated flows under confinement. While the central role of nematic defects as sources of active flows and pattern formations is well-established, the feedback of vortical flow on the nematic field is not well understood. Furthermore, the majority of research has focused on two-dimensional flows, simulating the model experimental kinesin/microtubule-based active film system; however, three-dimensional (3D) active nematics have recently been realized [1]. To untangle the complex active flow states in 3D, we propose a method that illuminates underlying structures in the orientation of the flow field to localize the eye of vortices. By performing numerical simulations of confined and bulk 3D active nematic fluids, we characterise the pattern formations of orientational defects in the nematic and flow fields (Figure 1). Our results show how active turbulence in the bulk is sustained by a complex and dynamical network of nematic disclination lines that either grow to span the system size or shrink until self-annihilation [2, 3]. In contrast, the contour lengths of singular flow lines are distributed about a characteristic length, independent of the system size. By studying the spatiotemporal structure of flow/nematic singularities and their interplay, we provide a complementary perspective on active liquid crystalline dynamics.

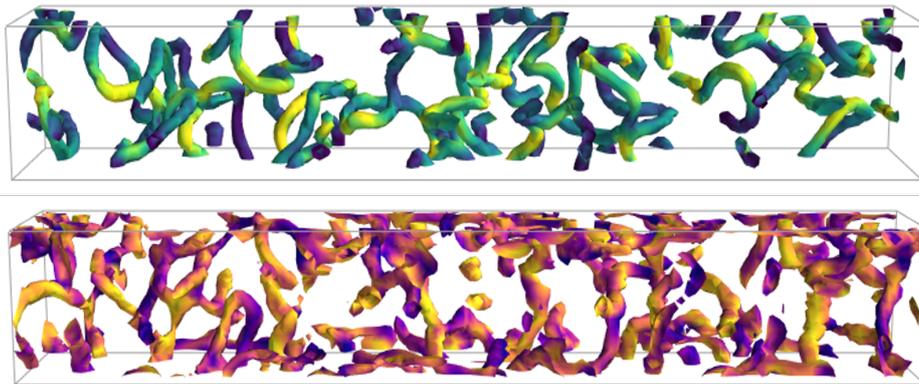


Figure 1: Disclination lines in the director field [4] (top) and velocity orientation field (bottom).

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Towards chemical sensing applications using chiral nematic liquid crystal droplet lasers

J. Norman, P.J.W Hands*

Institute for Integrated Micro and Nano Systems, University of Edinburgh, Edinburgh, EH9 3FF, UK

*Philip.Hands@ed.ac.uk

Chiral nematic liquid crystal (N*LC) droplets have been identified as a high potential chemical sensing platform due to their optical response to analyte-induced changes in droplet surface anchoring and adaptability to different applications [1, 2]. However, most sensors so far reported rely on manual and qualitative interpretation of images, although attempts have been made to create quantitative outputs through image analysis algorithms [3].

We present the latest efforts to enhance LC sensing using dye-doped N*LC (DDN*LC) droplet lasers packaged within a purpose built lab-on-chip device. Exploiting a bandedge lasing mechanism, emission from DDN*LC droplets provides a quantitative and multi-metric alternative to image-based detection. Poly(vinyl alcohol) (PVA) and Sodium Dodecyl Sulfate (SDS) were used to promote planar degenerate and homeotropic droplet surface anchoring respectively, with the laser emission characterised during planar to homeotropic realignment. Starting in a Bragg onion configuration with omnidirectional lasing, subsequent changes in emission intensity and wavelength were identified which corresponded to the SDS concentration used.

It is anticipated that with development in functionalising DDN*LC droplet surfaces for specific sensing applications, combined with recent advances in LC lasers [4], DDN*LC droplets could provide a promising avenue for integrated LC sensor devices with an automated and quantitative output. In addition, bandedge laser emission could potentially be more readily measured and simpler to instrument compared to other LC droplet laser mechanisms which have been applied to sensing [5].

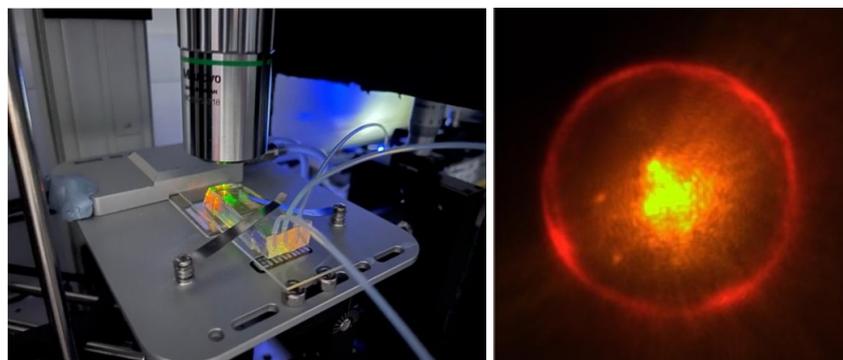


Figure 1: Images of lab-on-chip device developed for droplet laser sensing (left) and a lasing DDN*LC droplet following introduction of SDS surfactant simultaneously demonstrating a bright central bandedge lasing spot and peripheral whispering gallery mode lasing (right)

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Enantiomers Self-Sort into Separate Counter-Twisting Ribbons

X.B. Zeng^{*a}, Y. Wang,^b Y.X. Li,^c L. Cseh,^d S.G. Yang,^b R.B. Zhang,^a F. Liu,^b G. Ungar^{a,b}

^a Department of Materials Science and Engineering, University of Sheffield, Sheffield S1 3JD, UK.

^b State Key Laboratory for Mechanical Behaviour of Materials, Xi'an Jiaotong University, Xi'an, 710049, China.

^c School of Chemistry and Chemical Engineering,

Henan University of Technology, Zhengzhou 450001, China.

^d Romanian Academy, Coriolan Dragulescu Institute of Chemistry, Timisoara 300223, Romania

*x.zeng@shef.ac.uk

The recently discovered orthorhombic liquid crystal (LC) phase of symmetry $Fddd$ [1,2] is proving widespread, particularly in rod-like molecules with multiple chains attached at both ends (polycatenars). In this work the phase behaviour of hexacatenar compounds, containing a chiral hydroxybutyrate linkage in the core, has been studied extensively using a combination of standard and modulated differential scanning calorimetry (DSC), powder and grazing-incidence small- and wide-angle X-ray diffraction with electron density reconstruction, polarized microscopy with birefringence measurements, circular birefringence and dichroism spectroscopies (CB, CD) using Muller matrix method etc. The results show that while pure R and S enantiomers form only the Col phase, the racemic mixture forms a highly ordered $Fddd$ with 4 right- and 4 left-handed twisted columns traversing its large unit cell. In that structure the two enantiomers locally deracemize and self-sort into the columns of their preferred chirality. The twisted ribbons in $Fddd$, with a 7.54 nm pitch, consist of stacked rafts, each containing ~ 2 side-by-side molecules, the successive rafts rotated by 17° . In contrast, an analogous achiral compound with an achiral linkage forms only the Col phase. In spite of not forming a "proper" $Fddd$, pure enantiomers develop locally ordered $Fddd$ -like domains in the Col phase, as does the racemate above the Col- $Fddd$ transition. CB and CD spectra of enantiomers in the Col phase reveal strong induced chirality but without long-range order, hence "parachirality".

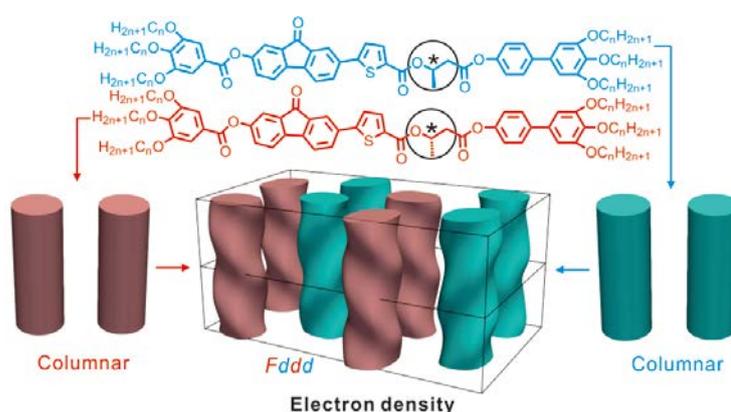


Figure 1. The R- and S- enantiomers of the hexacatenar compounds (top) form columnar phase only, but their racemic mixtures form a highly ordered $Fddd$ phase, with enantiomers locally deracemize and self-sort into 4 right and 4 left-handed twisted columns in the unit cell.

References

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Optical measurement of the twist elastic constant for nematic liquid crystals

D. Bankova^{*a}, N. Podoliak^a, M. Kaczmarek^a, G. D'Alessandro^b

^a School of Physics and Astronomy, University of Southampton, Southampton SO17 1BJ, UK

^b School of Mathematical Sciences, University of Southampton, Southampton SO17 1BJ, UK

*d.o.bankova@soton.ac.uk

Liquid crystals (LCs) have various applications, the most widely known of which is display technologies. As the LC response depends on several parameters including the elastic constants, determining the elastic constants is important for the operation of liquid-crystal devices. Measuring the twist elastic constant K_2 is particularly important for devices in a twist-cell configuration. However, measuring K_2 is not as easy and accurate as measuring the splay K_1 and bend K_3 elastic constants.

We have used a Cross-Polarised Intensity (CPI) method for measuring the splay and bend elastic constants, viscosities, cell thickness, pretilt and polar anchoring energy [1-3] in planar LC cells. Here we extend this method to twist LC cells for the measurement of the twist elastic constant K_2 (see Figure 1).

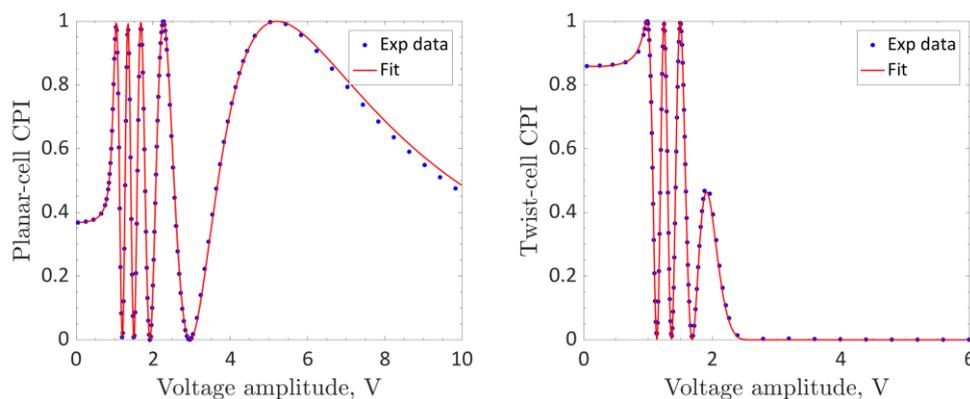


Figure 1. Planar-cell (left) and twist-cell (right) mean cross-polarised intensity for 5CB cells as a function of the applied voltage. By fitting these measurements we estimate that the elastic constants of 5CB at room temperature are $K_1=5.6$ pN, $K_2=3.4$ pN and $K_3=7.8$ pN.

We use a non-standard configuration of crossed polarisers and a twist LC cell. This allows us to measure accurately the twist elastic constant by reducing the degeneracy of K_2 and the cell thickness. The non-standard setup combined with a numerical model based on an effective beam propagation method [4] give a new reliable optical method for measuring the twist elastic constant of nematic liquid crystals in standard twist LC cells.

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Order parameter modelling using molecular simulation techniques

G. Zhao^{*a}, T. Le^a, M. R. Wilson^b and A. J. Masters^a

^a Department of Chemical Engineering, University of Manchester, Manchester M13 9PL, UK

^b Department of Chemistry, University of Durham, Durham DH13LE, UK

*guinan.zhao@postgrad.manchester.ac.uk

Order parameter modelling is used to model a nematic liquid crystal at the mesoscale. Typically such models make use of an underlying Helmholtz energy functional, expressed in terms of the \mathbf{Q} -tensor. To obtain the equilibrium state of the nematic, the Helmholtz energy is minimised with respect to \mathbf{Q} . Generally, the minimisation is carried out numerically over a set of grid points. Order-parameter modelling methodology has been used to study a wide variety of liquid crystal devices, the properties of colloidal particles suspended in a nematic host and much more besides.^[1]

To model more complex liquid crystals, such as biaxial smectic or banana phases, one has to deal with an increased number of degrees of freedom and numerical minimisation of a Helmholtz energy functional on a grid becomes more problematic. For such systems, a particle-based or Lagrangian formulation has its attractions, where an average over particle positions and orientations can yield the required information.

Here we propose the application of many body dissipative particle dynamics (MBDPD) techniques^[2] to liquid crystals. The underlying Helmholtz energy functional is converted into a potential energy function. Standard molecular Monte Carlo and molecular dynamics techniques are used to track particle motion, whereupon an ensemble or time average yields the required properties. No sophisticated numerical minimisation techniques are needed, so one may study functionals with many degrees of freedom, such as have been proposed for the phases of bent core particles.^[3] Here we provide a proof of principle of this technique by applying it to the nematic phase. We show that we can successfully model nematic behaviour, including the effects of an external field, anchoring and elastic deformations. We do not believe that our suggested methodology will be competitive with existing techniques for nematic phase modelling, but we do suggest that this study paves the way for its use in the modelling of more exotic liquid crystals in complex geometries, obviating the need for complex numerical methods.

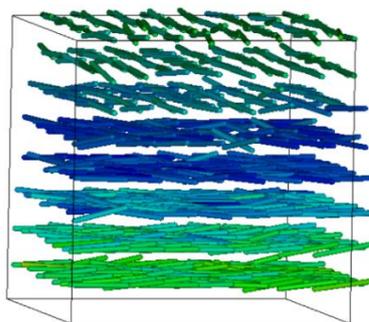


Figure 1. A snapshot of a twisted nematic cell from an MBDPD simulation.

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Making light with liquid crystals:

Luminescent LCs via ionic self-assembly and supramolecular interactions

S. Laschat^{*a}, A. Zens^a, F. Giesselmann,^b A. Köhn,^c J. Kästner,^c Y. Molard,^d E. Zysman-Coleman^e

^a *Institut für Organische Chemie, Universität Stuttgart, D-70569 Stuttgart, Germany*

^b *Institut für Physikalische Chemie, Universität Stuttgart, D-70569 Stuttgart, Germany*

^c *Institut für Theoretische Chemie, Universität Stuttgart, D-70569 Stuttgart, Germany*

^d *CNRS, ISCR – UMR 6226, ScanMAT – UAR 2025, Univ. Rennes, F-35000 Rennes, France*

^e *Organic Semiconductor Centre, University of St. Andrews, St. Andrews, KY16 9ST, U.K.*

*sabine.laschat@oc.uni-stuttgart.de

With respect to energy efficiency there is an increasing demand for novel luminescent materials that can be applied for sensing, switching, lighting and energy conversion devices. Attractive candidates for this purpose are luminescent organic or hybrid liquid crystals due to their anisotropic order, easy solution processing, self-healing of defects and tunable emission colour. On the other hand several challenges exist, such as tedious synthesis, limited thermal, oxidative and photostability, reduced lifetime and moderate light efficiency. Some strategies to overcome these challenges will be presented. It will be showcased for merocyanines [1], flavylum ILCs [2,3], and clustomesogens derived from crown ethers [4,5] and guanidinium salts [6] that convergent synthesis, ionic self-assembly and supramolecular interactions provide convenient access to highly emissive LC materials. Furthermore, recent work on star-shaped mixed disk-rod mesogens [7] revealed that the orientation of the chromophore in thin films is controlled by the mesophase, which enabled the preparation of OLED devices.

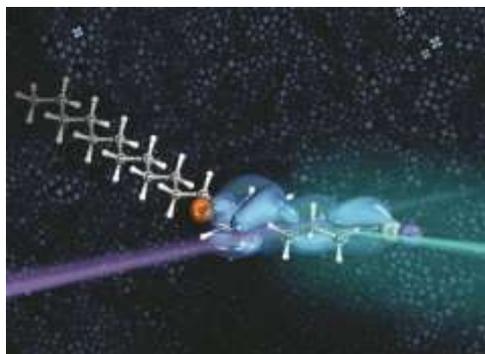


Figure 1. Structure of emissive liquid crystalline merocyanine with HOMO orbitals from DFT calculations. In the background Maltese cross textures from POM studies are shown. The figure was taken from ref. [1]

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Triphenoxazoles substituted with halogens: *Luminescent, liquid crystalline materials*

Michael S. Butlin^{1*}, Gregory C. O'Callaghan¹, Owen M. Jones¹, Karolis Viržbickas¹, Dennis Zhao¹, Alex P. G. Robinson² and Jon A. Preece¹

¹ School of Chemistry, University of Birmingham, UK, B15 2TT

² School of Chemical Engineering, University of Birmingham, UK, B15 2TT

*mx385@bham.ac.uk

Triphenoxazoles are hexalkoxytriphenylene based organic dye molecules with large *pseudo* Stokes shifts, high brightness and the ability to form thermotropic columnar hexagonal mesophases (Col_h).¹ A series of phenyl functionalised triphenoxazoles substituted with halogens (**TpOx-Ph-Hal**) were synthesised for the purpose of examining the effect of electron withdrawing group substitution pattern on the triphenoxazole emission spectrum and formation of the Col_h mesophase.

The luminescent properties were investigated with absorption and emission spectroscopy and the molar absorptivity, quantum yield and lifetimes were recorded. The *pseudo* Stokes shift was found to correlate strongly with the Hammett constant of the parent halobenzoic acid leading to predictive power when designing new emissive dyes.² The thermotropic liquid crystalline properties of the **TpOx-Ph-Hal** materials were characterised by polarising optical microscopy and differential scanning calorimetry with the transitions found to be influenced by the halogen substitution pattern. The **TpOx-Ph-Hal** series was typically liquid crystalline above 90 °C. However, several compounds display a room temperature Col_h mesophase upon cooling from the isotropic phase.

In 2018 the triphenoxazoles were commercialised through the formation of University of Birmingham spinout company; ChromaTwist LTD, with the company named “one to watch” by the Nature Research Spinoff Prize. Ultimately the triphenoxazoles may find applications in the fields of fluorescence microscopy, flow cytometry, organic electronics (e.g. OLED and OPV) and security inks.³

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Colour Printing with Liquid Crystals

E. Kozlovska*, S. Klein,

Centre for Print Research, University of the West of England, Bristol, BS16 1QY

*Elizabete.Kozloska@uwe.ac.uk

Liquid Crystals are mostly used in display applications. The colour generated in displays is the result of a combination of colour filters, polarisers and the liquid crystal. To produce displays with a high yield, the production happens in clean rooms to avoid any contamination of the liquid crystal. In a display the colour is generated by the colour the colour filters. The liquid crystal acts as a light valve. Cholesteric liquid crystals or chiral nematics selectively reflect light when oriented appropriately. The pitch of the twist determines the colour. These are the same colours as it is found in butterfly wings, berries, and mother of pearl, or in Lippmann photography. Lippmann photography is a direct positive interference based photographic process. The image is a one off. We would like to print Lippmann images by introducing structural colour in between the layers of a Woodbury type. Woodbury type is a continuous tone photomechanical print where the tonal range is achieved by a relief plate, which is filled with pigmented gelatine. By introducing a liquid crystalline layer into Woodburytype, we will have a rewritable print, where the colour can be changed by an external field. As first steps, we are testing how the liquid crystal anchors to different substrates and how it behaves in a non-clean, that is in a printing environment. As substrate, we have used glass, gelatine, agar, and paper. We will present the first results.



Figure 1: Filipe Alves, 'Plastic Parrot', Lippmann plate

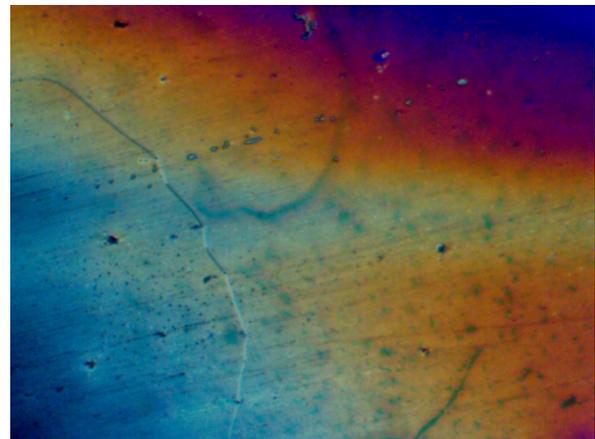


Figure 2: 5CB rolled onto agar substrate

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Liquid Crystal Laser Speckle Reducers

Nathan Spiller*, Yihan Jin, Chao He, David J. Hansford, Martin J. Booth, Steve J. Elston, Steve M. Morris
Department of Engineering Science, University of Oxford, Parks Road, Oxford, OX1 3PJ, UK
[*Nathan.spiller@eng.ox.ac.uk](mailto:Nathan.spiller@eng.ox.ac.uk)

Lasers are a highly desirable illumination source for imaging and display applications due to their high directionality, high intensity, and their potential to produce a wide colour gamut [1]. Additionally, their coherence properties enable optical diffraction-based imaging which is not accessible through conventional illumination sources, such as Ultra-High-Performance lamps and Light-Emitting Diodes. However, this coherence generates an imaging issue in the form of a spatially distributed granular distortion, termed speckle, which arises because of constructive and destructive interference when light is scattered [2]. Here we showcase liquid crystal (LC) based speckle reducers fabricated from short pitch chiral LCs that form a dynamic scattering mode (DSM) through electrohydrodynamic instabilities, which occur under certain electric field driving conditions [3-5]. To quantify the performance of the speckle reducers, a characterisation system has been developed to mimic the response of a human eye so as to record the speckle contrast parameter, C , as defined by J. Goodman [2]. By optimising the device architecture and material composition, through the addition of ionic dopants, redox dopants and/or zwitterionic dopants, the speckle contrast can be reduced to an almost imperceptible level, $C = 0.07$. This presentation will conclude with the demonstration of these LC speckle reducers in a range of applications including holography, microscopy, head-up displays (HUDs) and laser projection (Figure 1).

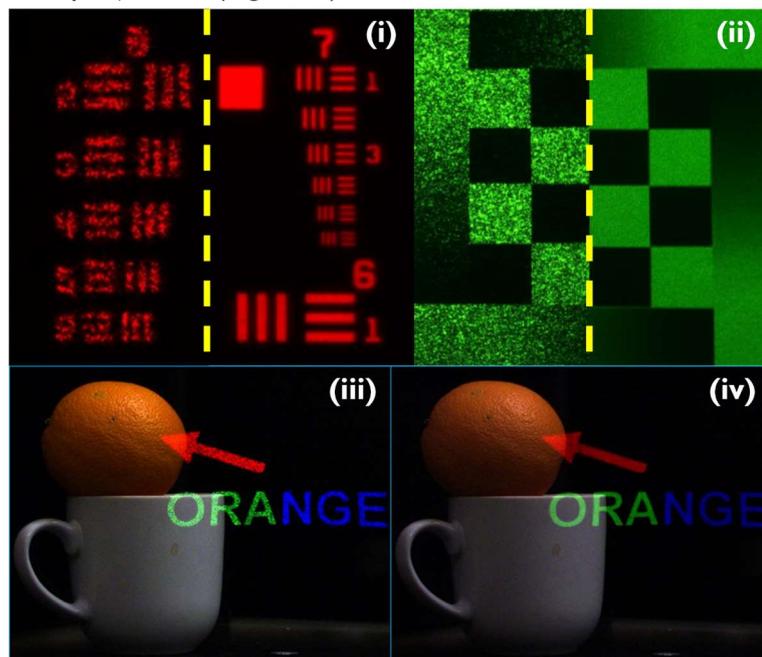


Figure 1: (i) Split image of a illuminated USAF target placed in a microscopy demonstrator: (Left) no speckle reduction, (Right) active speckle reduction from a LC device. (ii) Split image of laser projector output: (Left) no speckle reduction, (Right) active speckle reduction from a LC device. (iii) RGB laser HUD identifying a background object with no speckle reduction. (iv) RGB laser HUD identifying a background object with active speckle reduction from a LC device.

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The ferroelectric nematic phase – some history, some theory and some simulations

A. J. Masters^{*a}, D. Dunmur^b, M. R. Wilson^c

^a *Department of Chemical Engineering, University of Manchester, Manchester, M13 9PL, UK*

^b *Christ Church, University of Oxford, Oxford, OX1 2JD, UK*^b

^c *Department of Chemistry, University of Durham, Durham, DH1 3LE, UK*

*andrew.masters@manchester.ac.uk

In 2017, reports came through of the discovery of a ferroelectric nematic phase [1, 2]. A review of subsequent developments is given in [3]. Roughly a century earlier, Born had suggested that dipole-dipole interactions could generate such a phase [4]. Simulations of hard spherocylinders with embedded point dipoles, however, showed no sign of such ordering [5]. To obtain this phase, one clearly needs interactions that are not of the simple dipole-dipole form. We shall attempt to shed some light on what these interactions might be.

Firstly we give a historical summary of the controversy that arose from Born's conjecture. Secondly we report the results of molecular dynamics simulations on DIO-F, reported to form a ferroelectric phase [6]. These simulations indicate the growth of polar clusters from the isotropic phase.

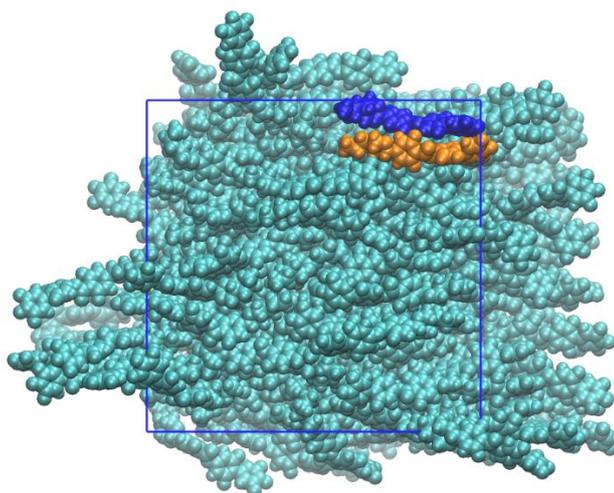


Figure 1. Ferroelectric clustering of DIO-F molecules

Finally we present both theoretical and modelling studies on hard, neutral spherocylinders with equal and opposite point charges embedded in the caps. In the presence of an electrolyte, where the Coulomb interactions are screened, we again show that there is a driving force for polar ordering.

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The Influence of Multiple Lateral Groups on the Formation of the Ferroelectric Nematic Phase

Cruickshank, Ewan^{a*}; Walker, Rebecca^a; Brown, Stevie^a; Storey, John MD^a and Imrie, Corrie T^a

^aDepartment of Chemistry, School of Natural and Computing Sciences, University of Aberdeen, Aberdeen, AB24 3UE, UK

The conventional uniaxial nematic phase, N, although the least ordered liquid crystalline phase, is at the heart of one of the most successful optoelectronic technologies, namely liquid crystal displays. Within the nematic phase, the constituent molecules align along a common direction known as the director, \mathbf{n} , whereas their centres of mass are randomly arranged. The director has inversion symmetry such that $\mathbf{n} = -\mathbf{n}$, and hence the phase is non-polar, **Figure 1 (a)**. The first reported experimental observations of a polar ferroelectric nematic phase, N_F , were reported in 2017 for RM734, [1] and DIO [2]. In the N_F phase there is a spontaneous alignment of the molecular dipoles and the inversion symmetry present in the N phase is lost, i.e. $\mathbf{n} \neq -\mathbf{n}$, and the phase is polar, **Figure 1 (b)**. The N_F phase has rapidly become the hottest topic in the field of liquid crystals not only because of its fundamental importance but also because of its true application potential.

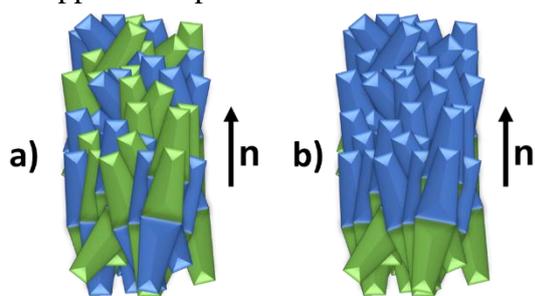


Figure 1. Schematic representations of the (a) conventional nematic, N, phase and (b) ferroelectric nematic, N_F , phase.

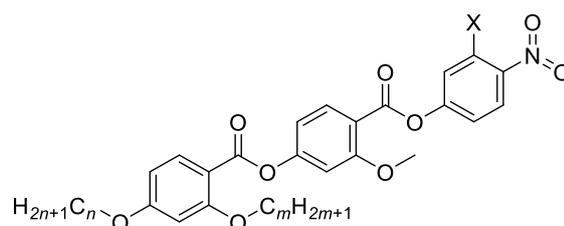


Figure 2. Molecular structure of the reported materials, where $n = 1, 2$; $m = 0-2$ and $X = \text{H}$ or F .

There are around 200 compounds to date which have been shown to exhibit the N_F phase [3-5] and improving the structural design of these materials requires a better understanding of structure-property relationships associated with the N_F phase but these remain at a very early stage. Here we report the transitional properties of a series of materials with a methoxy lateral group in the middle phenyl ring in which the ferroelectric nematic phase is observed, **Figure 2**.

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*Author for Correspondence: s02ec1@abdn.ac.uk

Differing phase behaviour of liquid crystal trimers containing *E* or *Z* benzanilides

G.J. Strachan,^{*a} E. Cruickshank,^a M. M. Majewska,^b D. Pocięcha,^b E. Gorecka,^b J.M.D. Storey,^a C.T. Imrie.^a

^a Department of Chemistry, University of Aberdeen, Aberdeen, UK

^b Department of Chemistry, University of Warsaw, Warsaw, Poland

*g.strachan@tcd.ie

Despite their ubiquity in organic chemistry, the amide group is relatively rare in low molar mass liquid crystals compared to groups such as esters and imines. Perhaps the most obvious role of an amide in liquid crystals is as a linking group to join two benzene rings within a mesogenic unit. Such a moiety is referred to as a benzanilide group and may be classed as secondary (2°) or tertiary (3°) based on their *N*-substituent. (Figure 1). The use of 2° benzanilides in smectic materials have been reported, which benefit from lateral hydrogen bonding between mesogens.[1–3] However, 3° benzanilides have proved difficult to incorporate into liquid crystals due to their strong preference for the *E* conformer, which dramatically alters molecular shape and disrupts liquid crystallinity.[4]

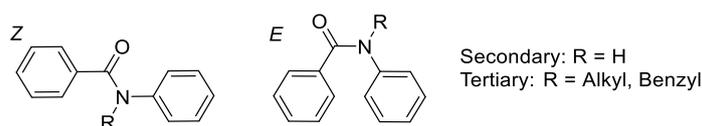


Figure 1. The *Z* and *E* conformations of the benzanilide group

Here we report the development of a molecular design in which both the *E* and the *Z* conformations are liquid crystalline. Secondary and tertiary benzanilide groups were used as the central mesogenic unit within a flexible trimer structure, and both sets of trimers formed a variety of nematic and smectic phases. However, the phase behaviour observed varied dramatically between structurally comparable 2° and 3° benzanilides. These differences reflect the dramatic influence that relatively small structural changes can have on liquid crystal phase behaviour.

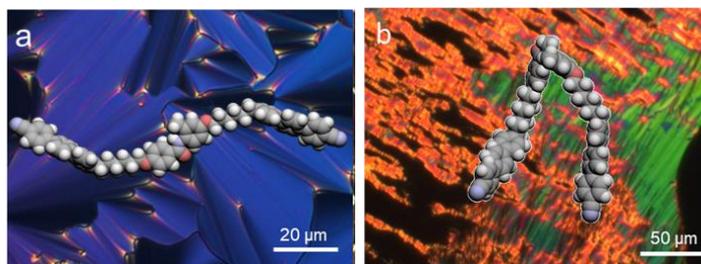


Figure 2. a) The *Z* conformation of a 2° benzanilide trimer and the POM texture of its smectic phase; b) a representation of the *E* conformation of a 3° benzanilide trimer and the POM texture of its smectic phase.

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Stepwise Twisting of Molecular Directions in a Double Gyroid Bicontinuous Cubic Phase

Y.M. Tang^a, R.B. Zhang^a, Y.N. Xue^b, X.B. Zeng^{*a}, G. Ungar^{*a,b}

^a Department of Materials Science and Engineering, University of Sheffield, Sheffield, S1 3JD, UK

^b State Key Laboratory for Mechanical Behaviour of Materials, Shaanxi International Research Centre for Soft Matter, Xi'an Jiaotong University, 710049, Xi'an, P. R. China

*x.zeng@sheffield.ac.uk; g.ungar@xjtu.edu.cn

Bicontinuous cubic (Cub_{bi}) liquid crystals (LCs) with homochiral interpenetrating infinite three-dimensional periodic networks are known to be generally found in the temperature region above the smectic and below the columnar phases.[1] Intriguingly, Cub_{bi} phase with $Ia\bar{3}d$ symmetry has been observed below the smectic phase for a series of polymers featuring polycatenar rod-like side-chain mesogen (Fig. 1a,b). Furthermore, different from the fact that successive rafts of several parallel mesogens prefer slowly uniform helical twist about the columnar segment axis in the same directions as demonstrated in previous instances, 3D electron density map of this phase suggests their successive rafts formed by the double layered polycatenar rod-like mesogen are not twisting continuously but in a stepwise, segmented style (Fig. 1c).[2-4] Other LC phases found in the vicinity of this Cub_{bi}/ $Ia\bar{3}d$ phase and their phase transitions will be discussed as well.

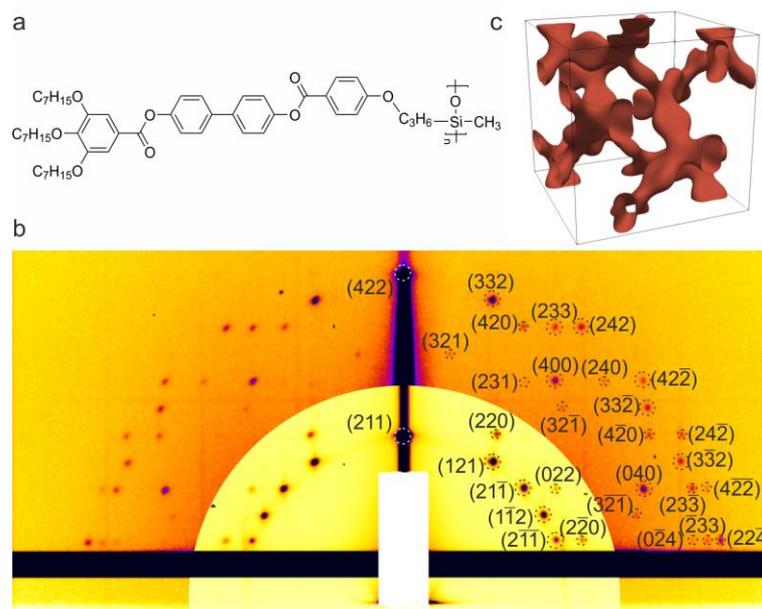


Figure 1. A thermotropic Cub_{bi}/ $Ia\bar{3}d$ LC phase formed from a polymer with polycatenar rod-like side chain. (a) Chemical structure of a representing compound; (b) the GISAXS pattern of the Cub_{bi}/ $Ia\bar{3}d$ phase, with diffraction peaks labelled by their Miller indices; (c) reconstructed electron density map of the phase. The red isoelectron surface encloses the high electron density region, showing stepwise twisting of molecular directions.

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Unusual applications of LC – mapping ultrasound fields

O. Trushkevych*^a, V. Reshetnyak^{b,c}, D.R Billson^a, D.A Hutchins^a, M Turvey^b, R.S. Edwards^b

^a School of Engineering, University of Warwick, Coventry, CV4 7AL, UK

^b Department of Physics, University of Warwick, Coventry, CV4 7AL, UK

^c Department of Physics, Taras Shevchenko National University of Kyiv, Kyiv, Ukraine

*o.trushkevych@warwick.ac.uk

Visualisation of acoustic fields is important in a range of fields, from aerospace and automotive industries, to materials research and nanotechnology. The standard method is to use laser vibrometry, which is a high-cost technique. Liquid crystal based acoustography [1] can also be employed for the task – this uses a thick layer of homeotropically aligned nematic LC between crossed polarisers and requires a setup in a water bath to aid acoustic propagation.

As an alternative, ultrasound can be visualised, potentially over a large area, using sensors based on polymer dispersed liquid crystals (PDLC) made of standard nematic LCs [2,3]. Visualisation using PDLC relies on the acousto-optic effect, where ultrasound interacts with the LC directly and visualisation of ultrasound is done via cleared areas of the PDLC. Acoustic field visualisation can also be done through thermal effects, arising from interaction of ultrasound and the sensor, with the help of chiral nematic (thermochromic (TLC)) liquid crystal films [4,5].

We demonstrate paint-on / removable PDLC sensors, discuss the mechanisms behind what we observe, and compare the sensing capabilities of PDLC and TLC. We explore capabilities of such passive film sensors in the context of non-destructive testing and structural health monitoring.

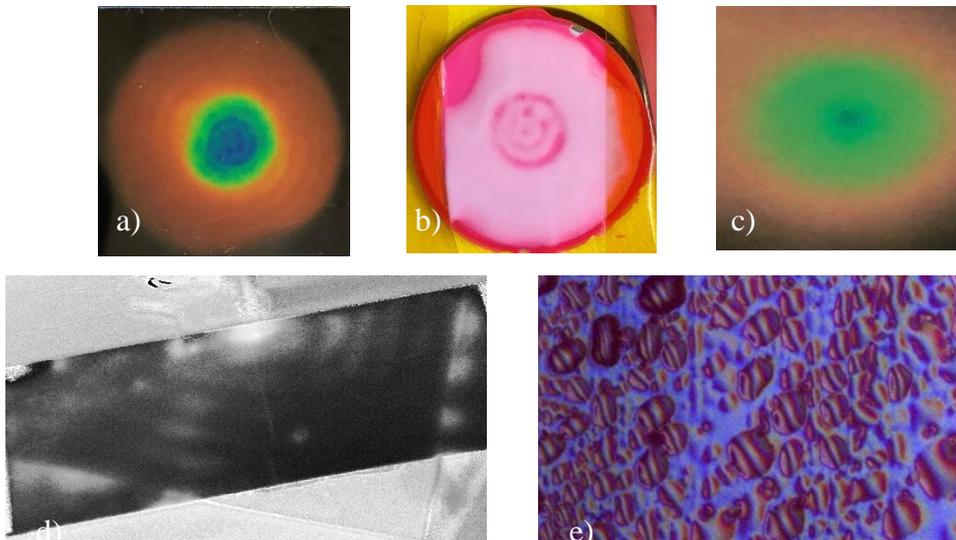


Figure 1. Visualisation of higher vibrational modes of an ultrasonic transducer a) using TLC sheet, 4.6 MHz, b) using PDLC coating, 6.7 MHz, c) fundamental frequency of the ultrasonic point probe at 40kHz, TLC sheet; d) standing Lamb waves on a thin plate, 40kHz, TLC sheet (the image was processed extracting hue for better visibility), e) polarised microscopy image of PDLC droplets under ultrasound excitation suggesting toroidal alignment of LC director inside droplets.

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Laser Written Liquid Crystal Vortex Beam Generators

C. Nourshargh*, P. S. Salter, M. J. Booth, S. J. Elston, S. M. Morris

Department of Engineering Science, University of Oxford, Parks Road, Oxford, OX1 3PJ, UK

*Camron.Nourshargh@eng.ox.ac.uk

We present a liquid crystal (LC) device capable of producing an optical vortex beam that is tuneable in both wavelength and orbital angular momentum (OAM) state. Through two photon polymerization direct laser writing, the director profile of a polymerizable LC can be structured in 3-dimensions [1-5] to form a 3-dimensional phase profile in space that converts an incident linearly polarized beam into a vortex beam of different orders (Figure 1). Importantly, the non-laser written LC regions remain electrically switchable after the laser writing process, enabling electrically tuneable 3-d phase masks to be produced. In this presentation, we demonstrate an optical vortex generator that can be electrically tuned to produce any integer or fractional optical vortex between zero and second order, for incident wavelengths ranging between 450-650 nm. Results from simulations are also presented that confirm the formation of the optical vortex beam and the phase profile is confirmed using a Mueller Matrix polarization imaging system.

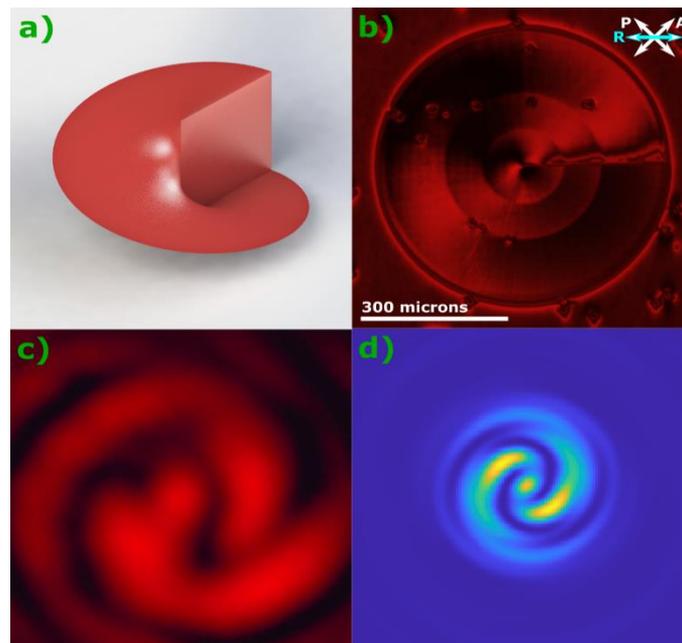


Figure 1: Overview of the laser written vortex beam generator. a) CAD model of the proposed structure, b) polarization optical microscope image of the laser written vortex beam generator, c) far-field pattern produced by the LC device in the absence of an applied voltage when the device aperture was overfilled, d) simulation of far-field pattern produced by the second-order vortex beam generator when the device aperture was overfilled.

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New investigations into the twist-bend smectic phases (SmC_{TB})

R. Walker^a, A.F. Alshammari^a, E. Cruickshank^a, A. Pearson^a, D. Pocięcha^b, J.M.D. Storey^a, E. Gorecka^b
and C.T. Imrie^a

^a Department of Chemistry, University of Aberdeen, Aberdeen, UK

^b Department of Chemistry, University of Warsaw, Warsaw, Poland

*rebecca.walker@abdn.ac.uk

Over a decade since they were first theorized,^[1,2] heliconical liquid crystal phases formed by achiral, bent-shaped molecules are one of the newest classes of liquid crystal phases and have recently attracted considerable global research interest. The twist-bend nematic phase, N_{TB} , is an intriguing and unique example of spontaneous mirror symmetry breaking in a fluidic state; a locally chiral phase formed from achiral molecules. In the N_{TB} phase, the director forms a helix and is tilted with respect to the helical axis; the spontaneous formation of chirality ensures that equal numbers of left- and right-handed degenerate helices are formed.^[3] More recently, heliconical twist-bend smectic C (SmC_{TB}) phases have also been discovered for liquid crystal dimers^[4,5] and in bent-core mesogens,^[6] and it appears that a range of variants of this phase, similar to the SmC^* subphases observed for chiral molecules, are possible.

Here we report the synthesis and extensive characterisation of several new homologous series of liquid crystals, showing rich liquid crystal polymorphism including twist-bend nematic and smectic phases, including the CB60_m series, phase behaviour of which is illustrated in **Figure 1**. Despite the molecules themselves being achiral, fascinating phenomena observed for these series include the transition between a phase with a single short helix and phase with a double helix, structural chirality at different length-scales and the exhibition of a photonic bandgap for visible light.

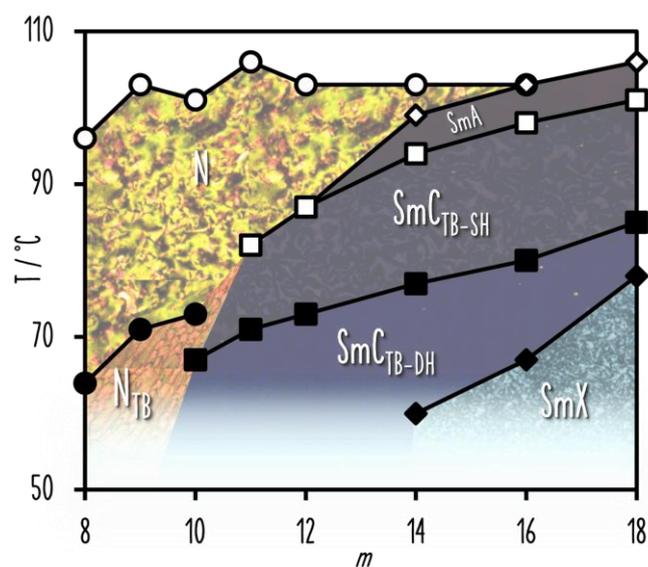


Figure 1. The dependence of the transition temperatures on the number of carbon atoms in the terminal chain for the CB60_m series.

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New examples of twist-bend liquid crystal phases

The synthesis and characterisation of the CBO6·Om series.

C. J. Gibb.^{1*}; C. Flores; J.M.D. Storey¹; D. Pocięcha²; E. Gorecka² and C.T. Imrie.¹

¹ Department of Chemistry, University of Aberdeen, Aberdeen, UK

² Department of Chemistry, University of Warsaw, Warsaw, Poland

c.gibb.18@abdn.ac.uk

Early research on liquid crystal dimers focussed on materials in which the flexible alkyl spacer was connected to both mesogenic cores by an ether-linkage (*OnO*). [1] The synthesis of *OnO* based dimers is typically straightforward and allows for a wide range of molecules to be synthesised quickly. More recently, and driven by the experimental discovery of the twist-bend nematic (N_{TB}) and heliconical twist-bend smectic (SmC_{TB}) phases in non-symmetric dimers, spacers connected by an ether and a methylene link (*nO*) have attracted increasing attention. [2-4] The synthesis of *nO* based dimers is more synthetically challenging than *OnO* based dimers, however research has focused on new synthetic methods to widen the types of materials that may be prepared. [5] For synthetic reasons, a comparison of a *nO*-based non-symmetric dimer with the corresponding *On* dimer has not been reported to date.

Here we present the synthesis and characterisation of the 1-(4-cyanobiphenyl-4'-yloxy)-6-(4-alkylanilinebenzylidene-4'-oxy)hexanes (CBO6·*Om*) which may be compared to the 1-(4-cyanobiphenyl-4'-yl)-6-(4-alkyloxyanilinebenzylidene-4'-oxy)hexanes (CB6O·*Om*) previously reported by Paterson *et al.* in which all 10 reported members exhibit the N_{TB} phase. [6] The CBO6·*Om* series are structural isomers of the CB6O·*Om* series in which the links connecting the spacer have been reversed. The CBO6·*Om* series are the first reported non-symmetric dimers to be synthesised in which this structural change has been implemented which has been achieved by utilization of a new synthetic pathway involving a variety of Pd and Pt catalysed cross-coupling reactions. In terms of their thermal properties, the two series behave similarly with differences in their values of $T_{N_{TB-N}}$ or T_{N-I} being statistically insignificant. Reversal of the spacer has a remarkable effect on the phase profile of the series, and although the N_{TB} phase is still exhibited by some members, the CBO6·*Om* series shows a range of fascinating smectic polymorphism including several SmC_{TB} phases.

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Measurement of chiral domain formation in N_{tb} thin films

S. L. Conopo-Holyoake^a, W. Jiang^a, C. Welch^a, G. Siligardi^b, G. H. Mehl^a

^aDepartment of Chemistry, University of Hull, Hull, HU6 7RX, UK

^bDiamond Light Source, Didcot, UK

g.h.mehl@hull.ac.uk

In previous work, it has been extensively reported by numerous researchers that the CBCnCB ($n = \text{CH}_2$ spacer units) series of molecules display a twist-bend nematic phase (N_{tb}). This phase is characterized by the emergence of chirality in non-chiral molecules and formation of helical structures, with a helical pitch ranging typically between 8-16 nm. The emerging chirality can be observed through the use of circular dichroism (CD) [1]. However, measurements of CD of thin films of liquid crystals are very often affected by positive interference of other optical properties, such as linear birefringence (LB), and linear dichroism (LD). Moreover, the LB and LD non chiral contributions are often much larger than CD giving rise to misleading interpretations. Typically this issue can be minimized by repeating the experiments after rotating and flipping samples, so that LB and LD are averaged out; ideally samples are oriented parallel to the CD beam, so that linear effects are at a minimum. [1,2]

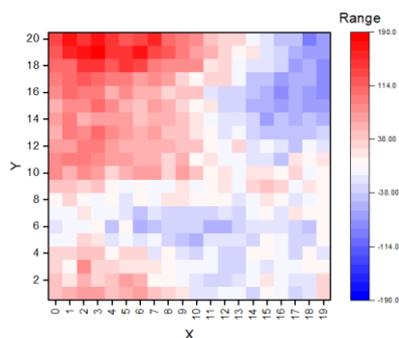


Fig. 1: CD mapping of CBC9CB across 1 mm² area of a 21x21 grid at 50 μm steps scanned at 510 nm and 115°C

Here we report the results of our experiments studying the characteristics of chiral domain clusters of the CBCnCB ($n = 7, 9, 11$) series in thin films at various temperatures. We show that the use of a dedicated nematic dopant achiral dye molecule admixed in small concentrations to the thin films, permits the recording of chirality beyond the absorption wavelength of the CBCnCB systems. Using the high resolution B23 beamline for Synchrotron Radiation Circular Dichroism (SRCD) and Mueller Matrix Polarimetry (MMP) at Diamond Light Source [3], we also conducted mapping experiments (see Fig. 1) across an area of the thin films, in order to visualise the formation of real chiral domains at the dopant-active wavelength. Using these results, we discuss the onset characteristics of chiral domain formation and compare this data with other results.

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Instabilities in liquid crystal elastomers

L. Angela Mihai^{*a}

^a *School of Mathematics, Cardiff University, Cardiff, CF24 4AG, UK*

*MihaiLA@cardiff.ac.uk

Liquid crystal elastomers (LCEs) are responsive multifunctional materials that combine the flexibility of polymeric networks with the self-organisation of liquid crystals. Due to their complex molecular architecture, they can exhibit dramatic spontaneous deformations and phase transitions, which are reversible and repeatable under external stimuli, such as heat, light, solvents, and electric or magnetic fields. These properties could be harnessed for a variety of advanced technological applications, including soft actuators, sensors, biomedical engineering and renewable energy. However, a better understanding of these materials is required before they can be exploited at an industrial scale.

Despite their difficult synthetic processes, the intriguing mechanical behaviour of LCEs has been probed extensively in laboratories around the world. Nevertheless, their constitutive characterisation can only be fully elucidated if integrated in a multiphysics framework combining elasticity and liquid crystal theories.

An important problem for both applications and our fundamental understanding of LCEs is their instability under large strains, as this can be useful in actuation, sensing, or patterning. The goal is then to identify parameter values at which a bifurcation emerges, and how these values change with external stimuli, such as temperature, or loads. Constitutive parameters of real manufactured materials have also an inherent variation that needs to be taken into account.

In this talk, I will present an overview of instabilities occurring in nematic elastomers [1–3], and examine the contribution of nematic order and fluctuating model parameters that follow probability laws. This mechanical analysis may lead to a more effective material characterisation of LCEs.

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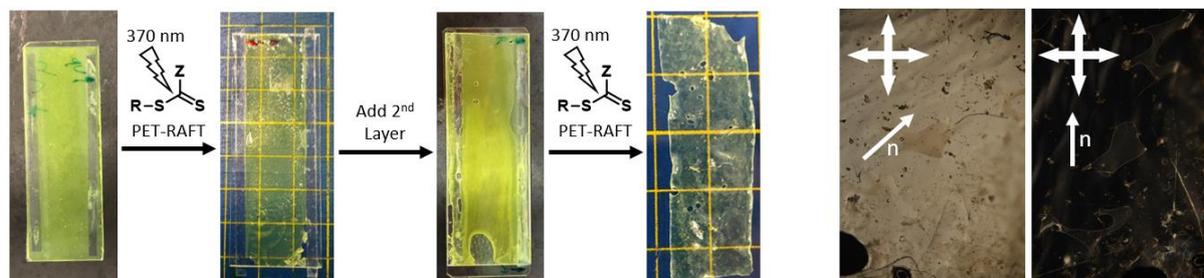
Increasing The Thickness of Surface Aligned Liquid Crystal Elastomers Through PET-RAFT Polymerisation

S. R. Berrow^{*a}, R. J. Mandle^{a,b}, H. F. Gleeson^a

^a School of Physics and Astronomy, University of Leeds, Leeds, LS2 9JT, UK

^b School of Chemistry, University of Leeds, LS2 9JT, UK

*S.R.Berrow@leeds.ac.uk



Liquid crystal elastomers (LCEs) are cross-linked polymers with low cross-link density, that combine the properties of elastomers (i.e. elasticity) and liquid crystals (i.e. self-organisation) [1]. They can possess several interesting properties, such as significant changes in shape/size upon application of stimuli [1-3], or auxetic behaviour [4].

The alignment of mesogens within the elastomer often determines the extent to which these interesting phenomena are observed [3,4]. Without attempts to align the mesogens, polydomain LCEs are isolated. These consist of microscopic domains of localised order, resulting in no overall macroscopic order in the sample. This lack of macroscopic order can eliminate or minimise the occurrence of phenomena such as auxetic or stimuli-responsive behaviours [3]. Consequently, the alignment of mesogens to yield monodomain LCEs, in which alignment is maintained throughout the sample, is desirable.

Several techniques have been developed to achieve monodomain alignment. One such technique is the use of surface alignment, which relies on mesogens interacting with surface coatings and in doing so being topologically aligned [2]. Surface alignment has many advantages over other techniques, such as enabling complex director patterns to be obtained [2]. However, the surface alignment technique is limited to low sample thicknesses (typically 100 μm), as the affinity for the mesogens to align decays with increasing distance from the alignment substrate [2].

Photoinduced electron/energy transfer reversible addition fragmentation chain transfer (PET-RAFT) polymerisation is a means of achieving living free-radical polymerisations [5]. It allows for a polymerisation to be stopped and started by the application or removal of a light source [6]. In this work, we present results that demonstrate the exploitation of this stop-start capability to produce monodomain LCEs of up to 300 μm thickness, aligned via surface alignment.

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Order and Optics of Liquid Crystal Elastomers

E.J. Cooper^{*}, M. Reynolds, T. Raistrick, D. Mistry, and H.F. Gleeson

University of Leeds, Leeds, LS2 9JT

**py17ejc@leeds.ac.uk*

The focus of research on liquid crystal elastomers (LCEs) has often been on their mechanical and physical properties, with potential applications including robotics and medical devices. Further proposed usages, based on the optical capabilities of LCEs, includes optical strain sensors and lenses [1]. Existing research on these optical properties of LCEs, typically involves measurements of birefringence [2] and refractive index modulation [3]. However, specific measurements of the ordinary (n_o) and extraordinary (n_e) refractive indices have rarely been reported, and techniques used so far include reflection spectroscopy [4], interferometry, and determination of Brewster's angle [5,6].

Recently, a new class of non-porous and transparent acrylate based LCEs were synthesized by Mistry et al [7] and discovered to exhibit auxetic behaviour. This family of LCEs has shown excellent capabilities as optical strain sensors [1], emphasising the potential of LCEs in the optics field.

This work reveals the role of composition on the order parameters of these acrylate-based and the subsequent impact of both order and composition on the refractive indices. Direct measurements of order parameters and refractive indices for a family of LCEs in which the mesogenic content was varied, were accomplished *via* Raman Spectroscopy and Abbe Refractometry, respectively. The mesogenic content of the LCEs was varied by 33 mol % and the nematic order parameter, P_2 , was subsequently found to range between 0.46 and 0.73. Furthermore, the refractive indices were found to notably differ following the alterations to composition and order parameters, wherein n_e displayed the greatest increase of approximately 0.026 for a 10 mol % increase in mesogenic content.

Understanding the optical properties of these transparent LCEs is key for understanding and designing optical applications of these materials.

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Direct and indirect evidence of biaxial order in auxetic liquid crystal elastomers

Thomas Raistrick^{*a}, Zhenming Wang^{a,b}, Aidan Street^a, Matthew Reynolds^a, Yanjun Liu^b, Helen F. Gleeson^a

^a School of Physics and Astronomy, University of Leeds, Leeds, LS2 9JT, UK,

^b Department of Electrical and Electronic Engineering, Southern University of Science and Technology, Shenzhen 518055, China

*phytr@leeds.ac.uk

Liquid Crystal Elastomers (LCEs) are weakly cross-linked polymer networks which contain mesogenic units. Recently, some LCEs have displayed an auxetic response when stretched, [1,2] which means that they become thicker when stretched. Until the discovery of auxetic LCEs, auxetic materials were made by designing porous structures into otherwise positive Poisson ratio materials. However, LCEs are auxetic on a molecular level, which has long been a goal of the auxetic community.

Auxetic LCEs, have been found to deform via a ‘mechanical Fréedericksz transition’, characterised by an apparent sharp rotation of the director at a critical strain, in contrast to the more typical ‘semi-soft elastic response’, where the director continuously rotates with applied strain. [3] The discontinuous nature of the ‘mechanical Fréedericksz transition’, together with measurements of the order parameters *via* Raman scattering, suggest that biaxial order may be important in auxetic LCEs. [2,4,5] We present direct evidence of biaxial order emerging in strained auxetic LCEs observed *via* conoscopic microscopy. [5] We show that the observations complement results from Raman spectroscopy, which probes the orientational order of the LCE as a function of strain, and reveal the emergence of biaxial order. Calculation of the orientational distribution functions shows that this facilitates the auxetic response *via* out-of-plane rotation of the mesogenic units. [2]

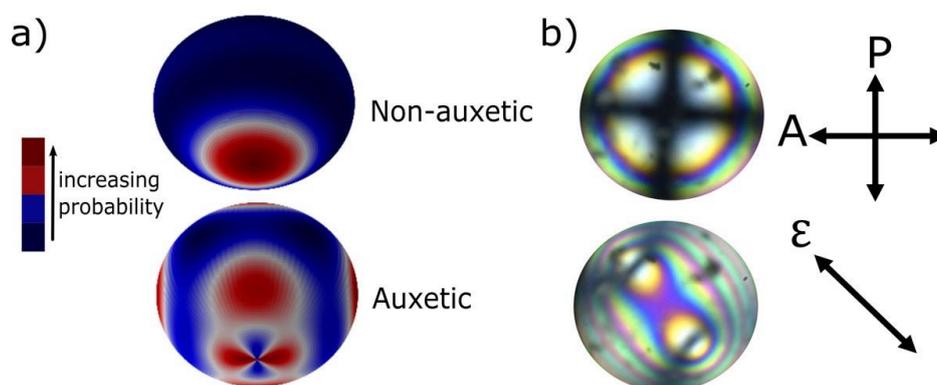


Figure 1. a) Orientational distribution functions of the LCE as determined *via* Raman spectroscopy suggesting the emergence of biaxiality due to imposed strains and out-of-plane rotations of mesogenic units. b) Direct evidence of biaxial order as determined *via* conoscopy.

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Geometrical control of colloidal liquid crystal alignment and dynamics

Ethan I. L. Jull^{*a}, Gerardo Campos-Villalobos^a, Marjolein Dijkstra^a, Lisa Tran^a

^a Soft Condensed Matter and Biophysics, Utrecht University, The Netherlands

*E.I.L.Jull@uu.nl

The shape, size, and anchoring conditions of a boundary determine the formation and structure of topological defects in confined liquid crystals. Micron-sized anisotropic biological systems are typically confined and exhibit liquid crystalline ordering, with defect structures mediating specific biological processes [1, 2]. Boundary anchoring control is then an essential tool for studying defects in micron-sized, liquid crystal systems. Prevailing chemical alignment techniques, commonly used in liquid crystal applications, cannot be leveraged for these larger-scale systems. However, geometrical control of rod orientation *can* apply across length scales [3, 4].

Here, we present experiments of a model, *pseudo-2D* colloidal liquid crystal. We probe the impact of confinement and geometrical boundary conditions on rod alignment and structure formation in nematic and smectic phases. We synthesised colloidal, micron-sized rods [5] with low gravitational lengths that are then confined in micro-cavities with varying geometrical features. We show the analysis of smectics confined by enclosing boundaries with varying curvature (Figure 1). The relationship between rod alignment and topographical features of the confining boundaries is also investigated, with an anchoring transition expected to occur for feature amplitudes and wavelengths of approximately the rod length and twice the rod diameter, respectively.

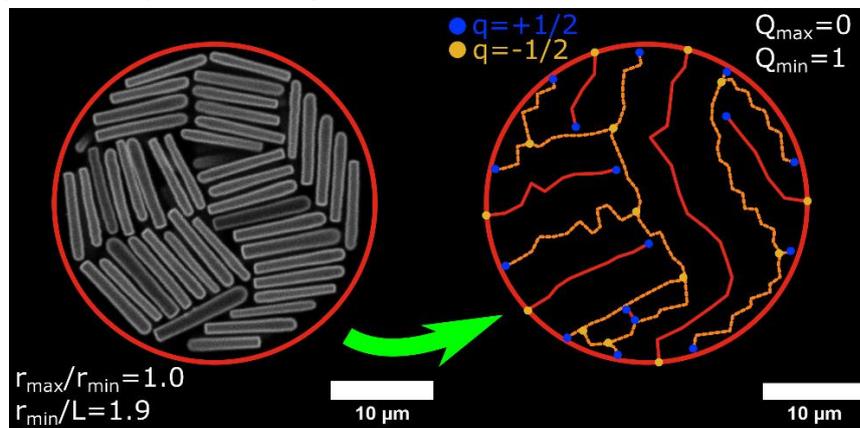


Figure 1. Colloidal particles in circular confinement form structures dependent on the confinement shape. Network analysis (right) of the smectic density maxima and minima is conducted to topologically classify and quantify the structures [6].

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On the flows of nematic liquid crystals through a T-junction

Kamil Fedorowicz^{*}, Robert Prosser

*Department of Mechanical, Aerospace & Civil Engineering, The University of Manchester,
Manchester M13 9PL, UK*

^{*}kamil.fedorowicz@manchester.ac.uk

Microfluidics devices are low-footprint instruments that combine and automate several laboratory processes. Initially, the microfluidic apparatus used Newtonian fluids and its applications were limited to biochemical sensors. The functionality of microfluidic devices can be improved by incorporating nematic liquid crystals. These consist of anisotropic molecules, which arrange into systems with long-range orientational order, and the mean local orientation is called the director [1]. Compared to isotropic fluids, the material anisotropy of liquid crystals results in several unique properties, e.g. variable viscosity, backflow, birefringence and anisotropic electrical permeability. These characteristics are exploited to manufacture novel microfluidic devices such as colour filters, velocimetry and flow tuning devices [2].

We use our recently developed OpenFOAM solver [3] to investigate the three-dimensional flow of nematic liquid crystals through a T-junction with homeotropic anchoring imposed on all walls. The geometry is a precursor for more complex microfluidic domains that are applied in mixing devices. Our results indicate a strong interplay between the flow and elastic effects when their strength is comparable. The flow contribution dominates in the inlet channel and causes the director to align with the flow in the upper part of the outlet channels (fig. 1). The flow stagnates at the lower wall below the inlet channel, and the location promotes the director alignment in the z -direction as imposed by the homeotropic boundaries. The varying director alignment is reflected in the velocity distribution; a two-stream profile is formed that is characteristic of binary fluids.

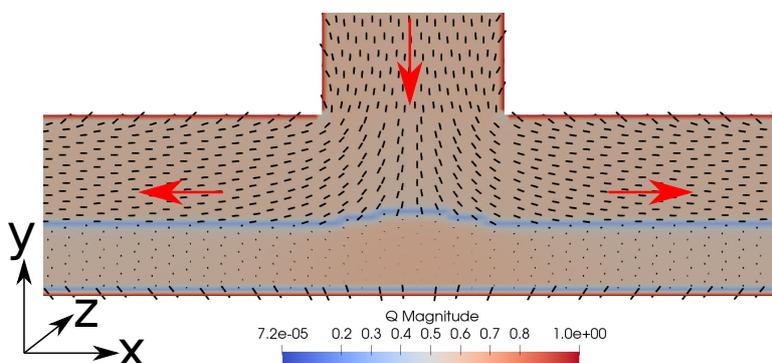


Figure 1: Contours of order parameter and glyphs of director field predicted by the Beris-Edwards model at $Er = 10$.

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The governing equations for a nematic liquid crystal Hele-Shaw cell

J.R.L. Cousins^{*a,b}, N.J. Mottram^a, S.K. Wilson^b

^a School of Mathematics and Statistics, University of Glasgow, Glasgow, G12 8QQ, UK

^b Department of Mathematics and Statistics, University of Strathclyde, Glasgow, G1 1XH, UK

*joseph.cousins@glasgow.ac.uk

A Hele-Shaw cell contains thin-film flow of fluid between parallel plates, where the lengthscale of the cell parallel to the plates is much larger than the lengthscale of the cell perpendicular to the plates. Flow in a Hele-Shaw cell is amenable to a thin-film (lubrication) approach, and significant progress is often possible using analytical methods and reduced models that are computationally cheaper than numerical alternatives [1]. Much of the previous work on Hele-Shaw flow has focused on isotropic fluids, and perhaps surprisingly, there has been relatively little work in the theory of Hele-Shaw cells filled with nematic liquid crystals (nematics), despite their relevance to the liquid crystal display (LCD) industry, where thin-film flows of nematics are a key element of LCD manufacturing. In the present work, we formulate and analyse a theoretical model for a nematic Hele-Shaw cell with a free fluid boundary $\partial\Omega$. In particular, we derive the thin-film Ericksen–Leslie equations, which govern the behaviour of nematic Hele-Shaw flow, and subsequently, consider the thin-film Ericksen-Leslie equations in the limiting cases of small and large Ericksen numbers in which we can make significant analytical progress. We demonstrate the use of the derived governing equations by analysing a common LCD manufacturing method called the One-Drop-Filling (ODF) method. In the ODF method, an array of nematic drops are squeezed between parallel plates inducing a thin-film flow which ultimately fills the device [2]. We consider a two-droplet ODF setup and obtain the nematic pressure, velocity and director in the limiting cases of small and large Ericksen numbers (as shown in Figure 1). We expect many other systems involving thin-film flows of nematic, including experiments on nematic viscous fingering [3] and nematic microfluidics [4], can also be analysed with the reduced models obtained.

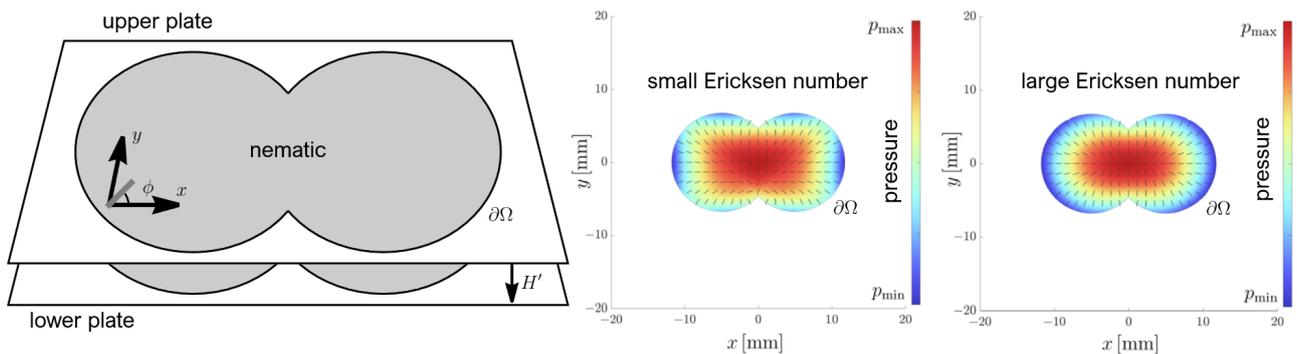


Figure 1: Schematic diagram of a two-droplet ODF setup. Plots of the nematic pressure with the director overlaid (shown by grey rods) obtained in the limiting cases of small and large Ericksen numbers are also shown.

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Liquid Crystal Alignment on Spontaneously Formed Surface Relief Structures

Thomas Moorhouse^{*1}, Erms R. Pereira¹, J. Cliff Jones¹

¹ School of Physics & Astronomy, University of Leeds, Leeds, UK

Controlling the surface alignment of the nematic liquid crystal (LC) director can be achieved via techniques such as mechanical rubbing or photoalignment, to induce anisotropic polymer orientation at a polymer-LC interface. Alternatively, grating aligned LC devices utilize topographically patterned surfaces, such as 1D, linear gratings. These typically micron-scale structures, can uniformly align the director [1] and also induce sufficient elastic distortion to facilitate bistable surface alignments; as seen in the Zenithal Bistable Display (ZBD) [2]. Fabrication of such structures is a non-trivial task often involving photolithography, interference lithography or electron-beam lithography, which are not at every researcher's disposal.

In this work, an entry level plasma cleaner is used to spontaneously form sub-micron scale, surface relief structures via a wrinkling phenomenon exhibited by plasma treated polydimethylsiloxane (PDMS) [3,4]. Nano imprint lithography is used to fabricate planar and homeotropic wrinkle-imprinted polyimide (WIP) surfaces, which are analyzed using atomic force microscopy (AFM) (Fig.1). A WIP surface with homeotropic anchoring results in an overall tilted alignment state, investigated using conoscopic and electro-optic approaches. Polarized microscopy observations indicate a surface anchoring transition to a metastable alignment state, supported by COMSOL multiphysics simulations, which suggest this transition is driven by the formation of surface defects. Confinement of this defect alignment state, by the walls of the pseudo 2D-grating structure of the WIP surface, results in a complex, periodic director profile; the textures and potential applications of which have been explored in this work.

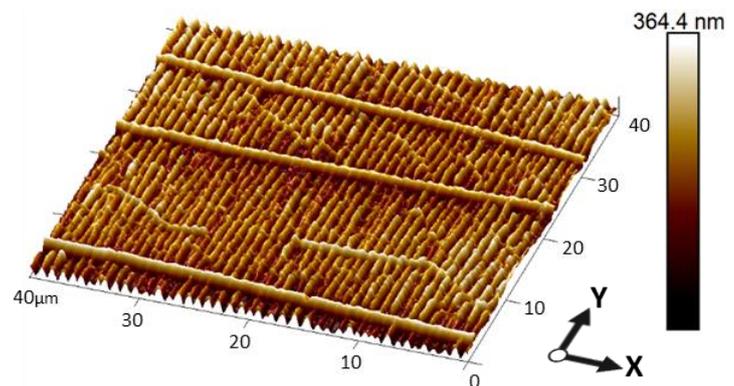


Figure 1: AFM scan of wrinkle-imprinted polyimide (WIP) surface. Periodic wrinkles parallel to Y and aperiodic walls parallel to X.

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* Author for Correspondence: py14tm@leeds.ac.uk

Surfing, sweeping and assembly of particles by a moving liquid crystal phase boundary

T. Shneer^a, J. Ochoa^{*b}, A. Wheeler^{*b}, B. Stokes^{*c}, L. S. Hirst^{*b} and T. J. Atherton^{*a}

^a *Department of Physics & Astronomy, Tufts University, Medford, MA, USA 02155*

^b *Dept of Physics, University of California, Merced, CA, USA 95343* ^c *Dept of Chemistry, Santa Clara University, CA, USA 95053*

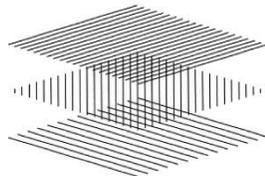
*timothy.atherton@tufts.edu

Nonequilibrium transport of particles embedded in a liquid crystal host can, by cooling through a phase transition, be exploited to create a remarkable variety of structures including shells, foams and gels. Due to the complexity of the multicomponent system and protocol dependent experimental results, the physical mechanisms behind structure selection remain only partially understood. Here we formulate a new model coupling LC physics to a Fokker-Planck equation as commonly used in studies of transport. The resulting model allows us to draw an analogy between the LC-nanocomposite system and chemotaxis, enriching the space of possible target structures that could be produced. We study the model in one dimension both analytically and numerically to identify different parameter regimes where soliton-like pulses of particles “surf” the interface or where the interface “sweeps” particles from one domain to another. We also consider an extended model that includes agglomeration of the particles and observe formation of periodic structures as a prototypical example of hierarchical self assembly. Results are compared with experimental observations of transport by isolated phase boundaries.

Poster Abstracts



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Astronomical Adaptive Optics Using Liquid Crystal Phase Modulators

O. Niculescu^{*a}, T.D. Wilkinson^a

^a *Department of Engineering, University of Cambridge, Cambridge, CB3 0FA, UK*

**on235@cam.ac.uk*

Adaptive optics is a technique used to reduce the effects of aberration on wavefront propagation. In Earth-based astronomy, this is used to correct for the light distortion which appears due to atmospheric turbulence. Customarily, for this application, adaptive optics systems use deformable mirrors as correctors, which are costly and mechanically actuated.

Correction is usually applied by phase conjugation, where any deformation introduced to the wavefront by the aberrating medium is then applied along the optical path with the inverse sign. Applying this correction requires the phase conjugate to be of the same amount as the aberration introduced, in a conjugate plane with the aberration source, and at a given time such that the deformation has not changed [1]. The layout of an adaptive optics system can be seen in Figure 1.

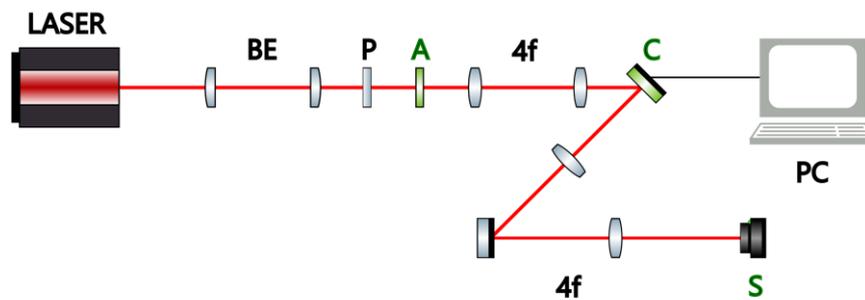


Figure 1. Schematic of the Adaptive Optics system, designed for testing reflective Liquid Crystal cells.

As opposed to a classic deformable mirror, which requires actuators to change its shape, a Liquid Crystal Wavefront Corrector (LCWFC) uses its inherent birefringence to act as a phase modulator and correct the incoming wavefront [2]. Despite its reduced size and cost, LCWFCs have historically suffered from a large response time [2], which makes them less desirable over a typical deformable mirror.

This work thus aims to use blue phase liquid crystal devices as the correcting element in the adaptive optics system. The blue phase of liquid crystals has been successfully stabilised for broad temperature use [3], and subsequently shown to be able to achieve very fast, polarisation-independent modulation of light on a silicon backplane [4], making it easily integrated with other electronic equipment for the fast correction of wavefront aberration.

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<https://doi.org/10.17863/CAM.36688>

Molecular Simulations of a New Class of Fluorescent Discotics

Arunkumar Bupathy*^a, Martin Walker^a, Mark R. Wilson^b, Dwaipayan Chakrabarti^a

^a *School of Chemistry, University of Birmingham, Birmingham B15 2TT, UK*

^b *Department of Chemistry, Durham University, Durham DH1 2LE, UK*

*a.bupathy@bham.ac.uk

Discotic liquid crystals, as a class of organic semiconductors in their self-assembled columnar phases, promise applications in opto-electronic devices, such as organic light-emitting diodes (OLEDs) and photovoltaic cells [1-3]. In this work, we undertake a computational study of a novel class of triphenylene derivatives, triphenoxazoles, recently synthesised [4]. These disc-like molecules comprise a triphenylene core with peripheral chains and a fused oxazole moiety, the latter having alkyl or aryl substituents, and display remarkable fluorescence characteristics [4]. We perform quantum chemistry calculations to interpret experimentally observed photophysical properties of this class of discotic mesogens. We also present results from our ongoing atomistic simulations to understand the phase behaviour of a prototype with insight into ordering at the molecular level and predict charge transport properties.

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Liquid Crystal Sensors for Ultrasonic Displacement Measurements

M.Turvey*^a, O. Trushkevych^b, D.J. McKnight^c, R.S. Edwards^a

^a *Department of Physics, University of Warwick, Coventry, CV4 7AL, UK*

^b *School of Engineering, University of Warwick, Coventry, CV4 7AL, UK*

^c *Pictura Bio, Wood Centre for Innovation, Quarry Road, Oxford, OX3 8SB, UK*

*m.turvey@warwick.ac.uk

Ultrasound field visualisation is important in the fields of non-destructive testing (NDT) and structural health monitoring, as it can be used to see where defects form in structures and components and how these defects progress over their lifetime. The standard method for wavefield visualisation is laser vibrometry, however, this can be slow and expensive due to the need for point-by-point scanning across the surface, and the cost to set up the equipment.

Previously, polymer-dispersed liquid crystals (PDLC) have been shown to allow fast and low cost visualisation of ultrasonic field displacement with a sharp on-off characteristic [1]. Thermochromic liquid crystal (TLC) films may be used in a similar way to map ultrasonic displacement, but with the potential to give a measure of ultrasonic displacement [2,3]. Heat generated by the ultrasonic field is absorbed by the TLC film, altering the pitch of the chiral nematic LC and resulting in a change in the wavelength of reflected light. This wavelength is determined from optical photography through comparison with a colour standard, and converted to temperature via a calibration curve. A temperature map is then used to give an approximation to the comparative displacement due to ultrasound vibration across the sample surface; temperature corresponds to several factors including displacement, environment, and thermal conductivity of the sample.

Here we use optical photography of the TLC sensors to measure temperature change across the TLC film when applied to a flexural ultrasonic transducer oscillating in distinct modal patterns at specific resonant frequencies (from 320kHz to 6.77MHz). Further displacement measurements were made using laser interferometry for comparison with the TLC data. A photo of the mode at 320kHz visualised by the TLC, temperature map analysis, and analysis of the displacement across the transducer as a function of angle is shown in figures 1(a)-(c). This shows the rings and unevenness of the modal pattern and matches the expected temperature range for the sensor.

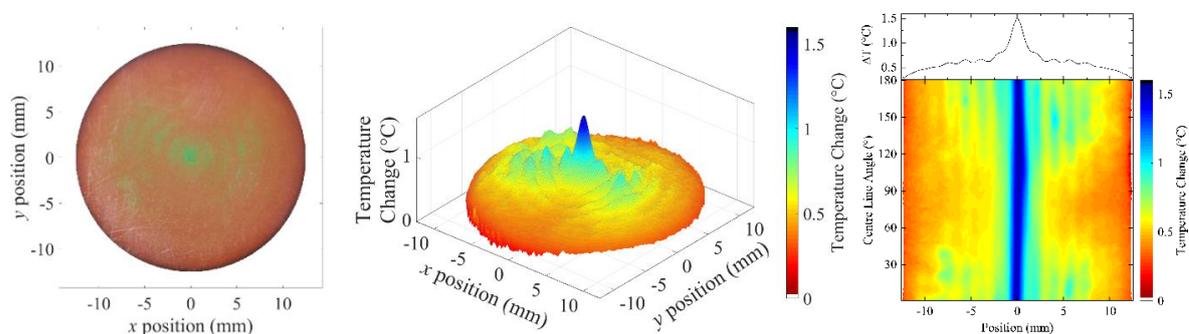


Figure 1. (a) Photo of the TLC sensor on the flexural transducer at 320kHz, (b) temperature map, and (c) the diameters from the temperature map, taken from 0 - 180° clockwise, with average temperature change (top).

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The structure of the ferroelectric nematic phase: insights from molecular dynamics simulations

Toby R. C. Thompson^a and Mark R. Wilson^{*a}

^a Department of Chemistry, Durham University, Lower Mountjoy, Durham, DH1 3LE, UK

*mark.wilson@durham.ac.uk

The reported experimental discovery of a ferroelectric nematic (N_F) phase is an exciting new development in liquid crystal research. It has potential applications in displays and novel technology due to its unprecedented polarization. This arises from large dipoles of N_F mesogens aligning in the same direction along the director (Fig. 1). The phase's origins are poorly understood, leading to derivatives of the first two mesogens to be discovered making up most of the known N_F mesogens [1].

Atomistic molecular dynamics (MD) simulations of liquid crystals can now reach timescales of hundreds of nanoseconds. Now that “real” molecules that exhibit the N_F phase are known, atomistic simulations are attractive for investigating the origins of phase formation. However, such calculations remain extremely challenging on the MD time scale [2].

Here we report on atomistic MD of an N_F mesogen: “DIO-F”. Optimisation of the force field is performed for DIO-F so that it can be simulated within the new GAFF-LCFF framework [3], which has been shown to deliver excellent transition temperature predictions. The N_F phase can be obtained both by rapidly compressing a box of aligned molecules and also by rapidly cooling an isotropic phase and then allowing the N_F phase to grow slowly over hundreds of nanoseconds. The normal nematic to N_F transition however remains out of reach, due to the slowness of molecular end-to-end rotation.

Different explanations for the stability of N_F are probed. Cylindrical distribution functions are observed to investigate the role of specific preferred intermolecular pairings. These are combined with densities of different phases to investigate claims that the mean excluded volume decreases as ferroelectric order grows [4]. Quantities including polarisation and orientation functions are compared between phases to judge the quality of the different methods used to generate the N_F phase.

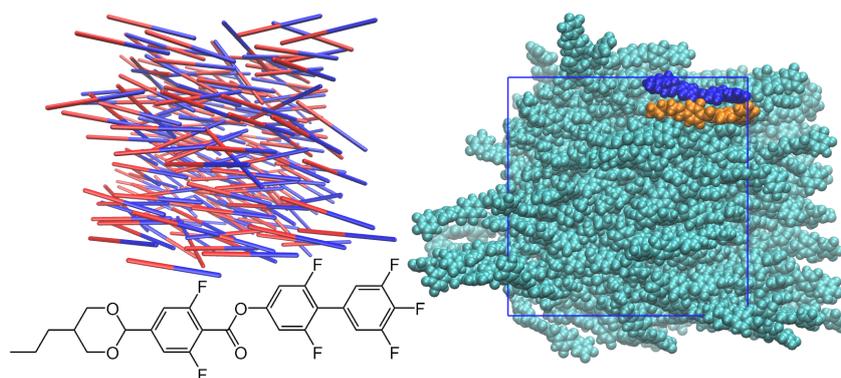


Figure 1: Visualisation of a ferroelectric nematic phase of “DIO-F “ generated with the fast cooling method.

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Improving the stability of liquid crystal lasers using a combined molecular-electromagnetic model

I. Pakamoryte^{*a}, D. Marenduzzo^b, N. Polydorides^a, P. J. W. Hands^a

^a School of Engineering, The University of Edinburgh, UK

^b School of Physics and Astronomy, The University of Edinburgh, UK

*ieva.pakamoryte@ed.ac.uk

Dye-doped chiral nematic liquid crystal lasers are a topic of increasing importance in soft-matter photonics. Broad wavelength tuneability (460-850 nm) and low cost and self-organising optical cavities make LC lasers extremely useful for a wide range of potential applications: for example, in fluorescence microscopy, enabling precise wavelength control for targeted fluorophore excitation; and in low speckle laser based imaging [1]. However, liquid crystal laser stability and power output are limited by several factors, including temperature, choice of materials, and pump pulse parameters. Pump pulse intensity and repetition rate (Fig.1) must be carefully controlled to avoid thermal excitation [2], optically-induced reorientation [3], and triplet state generation [4], although these are mostly temporary. In extreme cases, permanent degradation (i.e. photobleaching) of the dye is also possible.

A comprehensive study of the relative importance of the above effects under a variety of different experimental conditions has not been made. We will present a molecular-electromagnetic chiral nematic liquid crystal laser model, which we are developing to further investigate the molecular dynamics of dye-doped chiral nematic liquid crystal under the pump beam illumination over time. It is hoped that by fully understanding this parameter space, higher power lasers with stable performance can be produced, that are suitable for commercial applications.

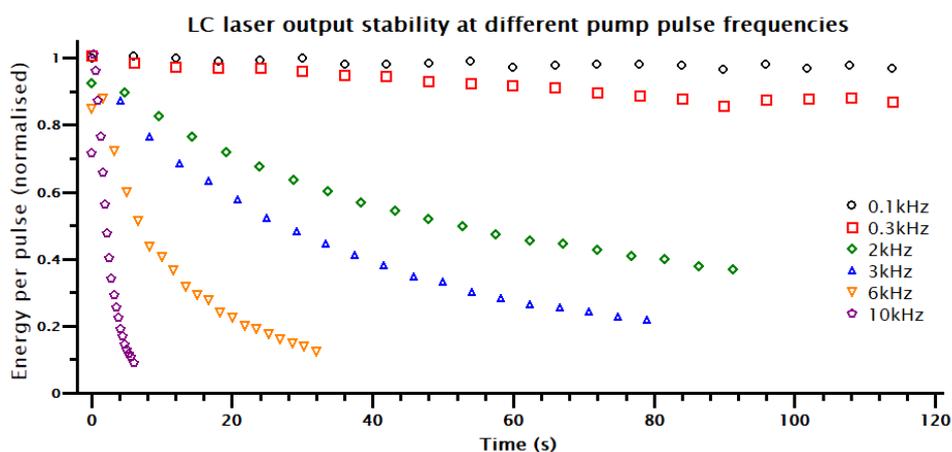


Figure 1: Experimental data illustrating the effect of pump beam repetition rate upon liquid crystal laser output stability. (Data replotted from [5]).

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Density Measurements of Liquid Crystals

Charles Parton-Barr^a, Helen Gleeson^a, Richard Mandle^{*a,b}

^a School of Physics and Astronomy, University of Leeds, Leeds, UK

^b School of Chemistry, University of Leeds, Leeds, UK

[*R.Mandle@leeds.ac.uk](mailto:R.Mandle@leeds.ac.uk)

Density measurements are a valuable tool for the study of phase transitions [1] and, in combination with x-ray diffraction, allow for the determination of molecular arrangement [2]. They play a role in the calculation of the optical and dielectric anisotropy of nematic liquid crystals through the Vuks and Maier-Maier relations [3]. We note that the assumption density, $\rho \approx 1 \text{ g cm}^{-3}$ does not necessarily hold true for all nematics.

We develop an experimental method that permits density measurements of liquid crystalline materials. The validity of this method has been ascertained through measurements of nematic (5CB (fig. 1a), (NCS)PCH6) and smectic (8CB) materials and comparison with existing literature values. The solid-at-room-temperature nematic RM2835 was measured with the aim of expanding the range of liquid crystals available to study.

The discontinuous change in density that occurs at the material's phase transitions is detected, indicating that the method is sensitive enough to provide meaningful data about the liquid crystal state. With regards to reliability, our results show excellent agreement with those previously obtained. While the method requires a large quantity of material (~1ml), it can be quantitatively recovered from the process

Experimental measurements of density are important for validating molecular dynamics simulations. If the quantum chemical calculations and molecular force field methods used lead to an inaccurate representation of the liquid crystal state it can result in errors, such as an increased level of stability for certain mesophases [4].

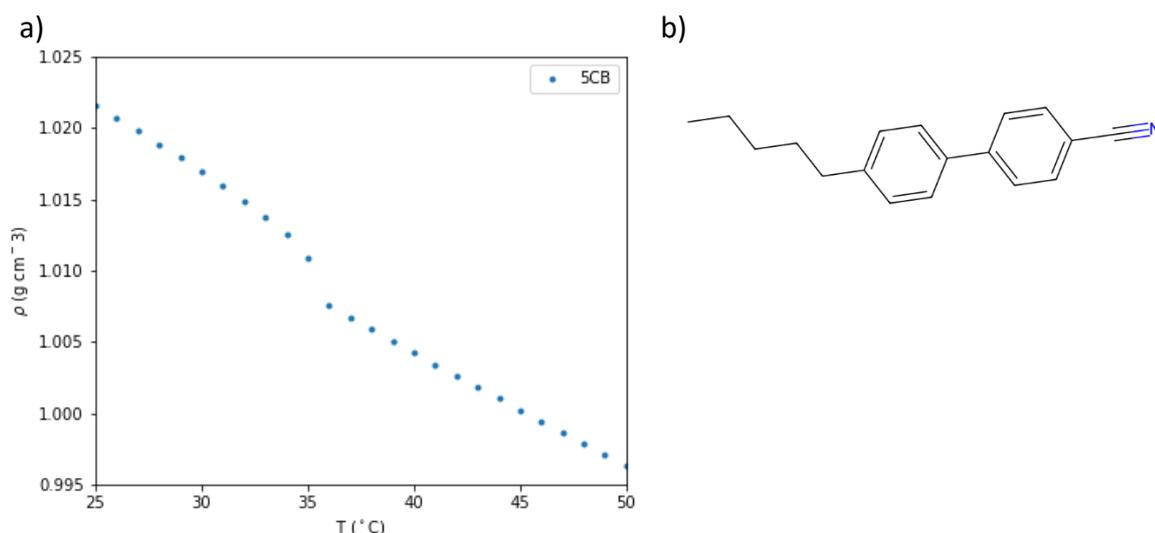


Figure 1. a) Density measurements of 5CB as a function of temperature. b) Structure of 5CB

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Structures for self-assembly of liquid crystal colloids

D. Shen¹, M. Afif¹, Z. Hong¹, F. A. Fernandez¹

*Dept of Electronic & Electrical Engineering, University College London, London, WC1E 6BT, UK
uceedsh@ucl.ac.uk*

Ordered arrays of nano- and micron-size particles are of much interest in many areas ranging from medical and chemical sensors, novel materials, displays, to photonics. It is also known that these arrays can be self-assembled from liquid crystal colloidal mixtures, which present an attractive route to fabricate these arrays [1-3].

Liquid crystals director patterns and defect structures induced by surface alignment and anchoring conditions and electric fields enable the capture of dispersed particles [4, 5].

We have been using LC modelling based on the Q-tensor to represent the LC orientation in the Landau-de Gennes theory [6, 7] to study several possible structures that can include different alignment conditions, surface relief patterns, and electrodes that can be utilised to produce these arrays. The objective is to generate adequate defect patterns that can be characterised by the strength and range of their attraction to dispersed particles.

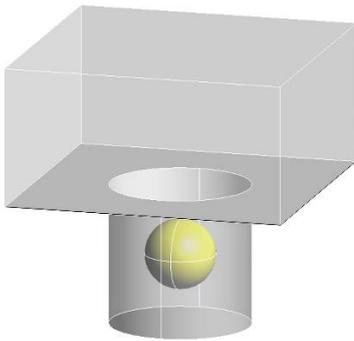


Figure 1: 3D view of one example of device structure for self-assembly.

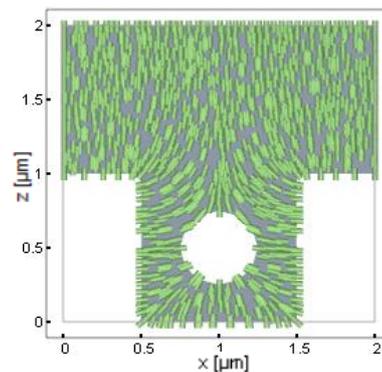


Figure 2: Cross-section showing director pattern around a particle in the lowest energy position.

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Alternative synthetic method to prepare liquid crystal dimers using sodium activated aromatic coupling reactions.

C. J. Gibb,^{1*} J.M.D. Storey¹ and Imrie, Corrie T.¹

¹ Department of Chemistry, University of Aberdeen, Aberdeen, UK

c.gibb.18@abdn.ac.uk

Recent research into the twist-bend nematic (N_{TB}) [1] and heliconical twist-bend smectic (SmC_{TB}) [2] phases has been focused on molecules containing aryl-alkyl and aryl-alkoxy links connecting the spacer to the mesogenic units. The preparation of these materials has largely involved traditional synthetic pathways that include difficult synthetic steps and often result in low overall yields and use expensive reagents.

Sodium activated aromatic coupling reactions help provide a cheaper, quicker and greener solution in the synthesis of more versatile intermediate compounds, ultimately allowing for more complex final materials. [3,4] By utilizing this one pot synthesis for 4-alkyl,4'-cyanobiphenyls and related units, it is possible to quickly create a library of liquid crystal dimers including the widely studied CB_nCB series as well as opening new avenues to previously challenging functional group chemistry. This reduction in synthetic steps has put new liquid crystal dimers and higher oligomers within reach.

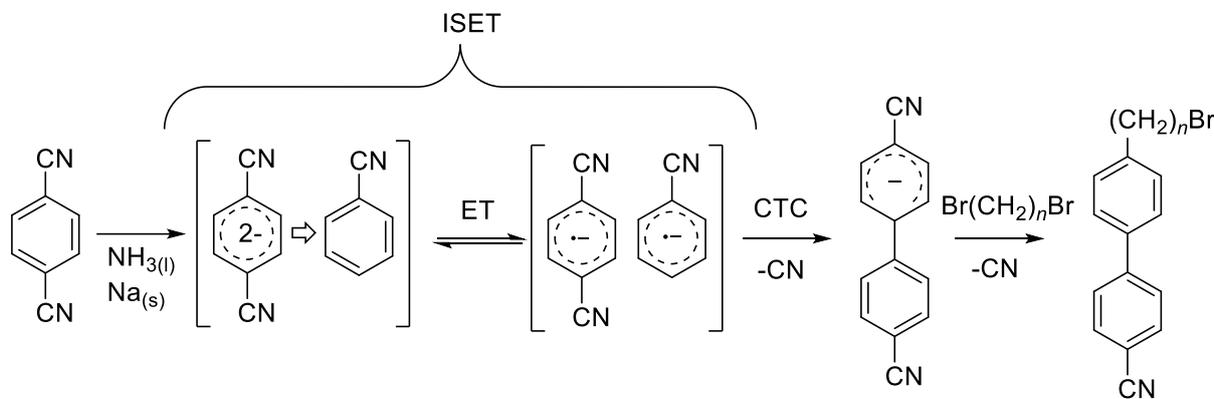


Figure 1. Proposed mechanism for the formation of versatile alkyl-4' nitrile biphenyls intermediates by sodium activated aromatic coupling reactions.

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The effect of varying terminal alkyl chain length on the ferroelectric nematic phase

Marijus Juodka^{*a}, Rebecca Walker^a, John MD Storey^a and Corrie T Imrie^a

^a Department of Chemistry, School of Natural and Computing Sciences, University of Aberdeen, Aberdeen, AB24 3UE *r01mj22@abdn.ac.uk

In the conventional non-polar nematic phase, N, molecules align themselves along the director (\mathbf{n}), described by a unit vector with inversion symmetry, i.e., $\mathbf{n} = -\mathbf{n}$. In 2017, RM734 and DIO became the first materials to exhibit nematic behaviour having spontaneous polarisation.[1,2] Further studies revealed a ferroelectric character to the lower temperature nematic phase in these materials, giving rise to the ferroelectric nematic phase, N_F , in which $\mathbf{n} \neq -\mathbf{n}$. [3] Despite their chemical structures being quite different, both have a large longitudinal molecular dipole moment, and this is thought to be fundamental for the formation of the N_F phase. This aside, the relationships between molecular structure and formation of the N_F phase are not yet well understood.

Modifications to the RM structure have been recently reported[4,5], whereas variations to the DIO structure have been explored to a lesser extent. Thus, here we present a study of the impact of the terminal alkyl chain length on the ferronematic properties of DIO (see **Figure 1**). Part of the synthetic method to make DIO is the formation of a 1,3-dioxane ring. The current literature method yields a 1:4 mixture of *cis/trans* isomers of the ring.[6] Notably, DIO exhibits liquid crystalline behaviour only with a *trans*-1,3-dioxane present in its structure.[6] Increasing the length of the terminal alkyl chain results in such isomers becoming harder to separate using conventional methods of purification such as flash chromatography. Thus, we have developed a novel synthetic approach that allows a degree of control over the isomer formation ratios depending on the temperature, concentrations of the reagents, and reaction time.

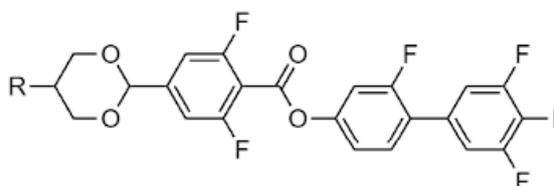


Figure 1. Target compounds of this study, $R = C_nH_{2n+1}$.

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Study of the Effects of Sulfur and Fluorine on Ferroelectric Nematic Liquid Crystals

Gytis Stepanafas^{*a}, Ewan Cruickshank^a, John M. D. Storey^a, Corrie T. Imrie^a

^a Department of Chemistry, University of Aberdeen, Old Aberdeen, Aberdeen, UK

* r02gs21@abdn.ac.uk

The nematic phase (N) is the most fluid and the least ordered liquid crystal phase, in which the molecules are oriented more or less in the same direction along the director, \mathbf{n} . The N phase has inversion symmetry, such that $\mathbf{n} = -\mathbf{n}$, and therefore, the phase is non-polar. In 2017, two rod-shaped molecules RM734 [1] and DIO [2] (Figure 1) possessing a large dipole moment were shown to exhibit a unique phase. This was determined to be the ferroelectric nematic phase, N_F . [3] In this phase, $\mathbf{n} \neq -\mathbf{n}$, and the phase is polar. The N_F has high response sensitivity to an applied external electric field and this coupled with nematic fluidity [4] gives it exciting potential for applications in the next generation of optical or electro-optical LC display devices.

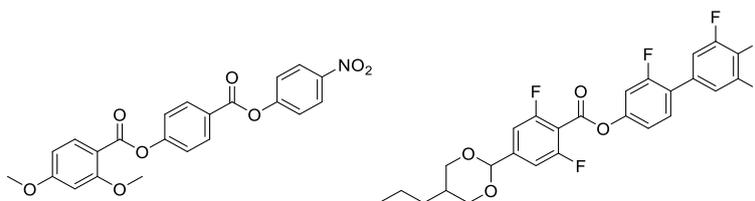


Figure 1 – Structure of RM734 (left) and DIO (right).

Here we report sulfur containing analogues of RM734 (Figure 2) in which the terminal ether link is replaced by a thioether to investigate the relationship between molecular structure and liquid crystalline behavior. Introducing a highly polarisable sulfur atom is expected to increase birefringence and extend the polarizable core of the molecule, whereas the addition of fluorine would enhance the N_F phase stability. [5,6] We report the corresponding materials with and without fluorine substituents to study the effect this has.

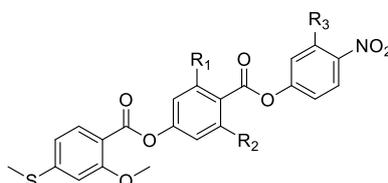


Figure 2 – Structure of sulfur containing RM734 analogues.

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Molecular Shape, Electronic Factors and the Ferroelectric Nematic Phase

N. Tufaha^{*a}, E. Cruickshank^a, D. Pocięcha^b, E. Gorecka^b, J.M.D. Storey^a, C.T. Imrie^a

^a Department of Chemistry, University of Aberdeen, Old Aberdeen, AB24 3UE, U.K.

^b Faculty of Chemistry, University of Warsaw, ul. Żwirki i Wigury 101, 02-089, Warsaw, Poland

*n.tufaha.21@abdn.ac.uk

Since the recent experimental discovery of the ferroelectric nematic phase, reported simultaneously by Mandle *et al.* [1] and Nishikawa *et al.* [2] in 2017, the phase has become the hottest topic in the liquid crystal community. Part of the interest in this newly found phase is the hope to develop a better understanding of its structure-property relationship and exploit its true application potential.

In contrast to the conventional uniaxial nematic phase, N, in which the constituent molecules align along a common direction known as the director, \mathbf{n} , with inversion symmetry $\mathbf{n} = -\mathbf{n}$, in the N_F phase, there is a spontaneous alignment of the molecular dipoles such that $\mathbf{n} \neq -\mathbf{n}$ and the phase is polar. Ester linkages, polar terminal groups or a high degree of fluorination result in a large longitudinal dipole moment which appears to support the formation of the N_F phase. [3]

Although suggestions have been made regarding the most efficient structural design for materials to exhibit the N_F phase [4,5], some recently reported examples have expanded these initial assumptions. [6] It is, therefore, critical that we now explore the effects that different structural modifications have on the stability of the N_F phase. Here we report the properties of two series of materials based on RM734 and the previously reported **5-*m*** and **6-*m*** series [7], namely the (4-nitrophenyl) 2-alkoxy-4-(4-methoxybenzoyl)oxybenzoates (NT3.*m*) and the (3-fluoro-4-nitrophenyl) 2-alkoxy-4-(4-methoxybenzoyl)oxybenzoates (NT3F.*m*) series, shown in Figure 1.

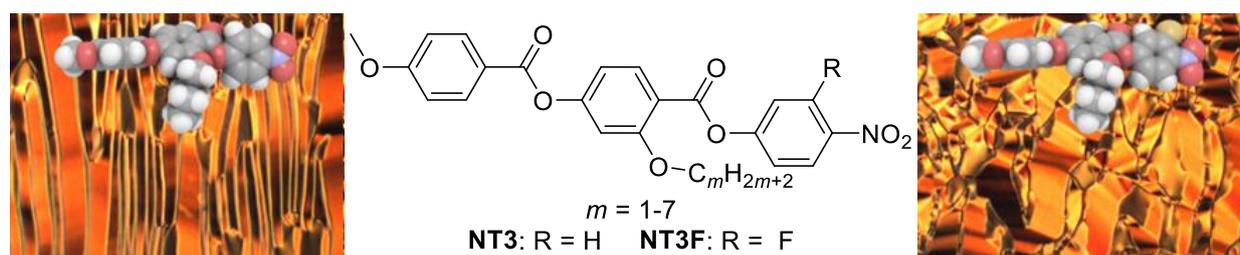


Figure 1. Molecular structure for the synthesised materials (middle), space-filling models and polarized optical microscope textures for N_F of respectively NT3.4 (left) and NT3F.4 (right).

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Auxetic Threshold and Order Measurements in two Liquid Crystal Elastomers (LCEs)

A. Street^{*a}, T. Raistrick^a, M. Reynolds^a, D. Mistry^a, & H.F. Gleeson^a

^a *School of Physics and Astronomy, University of Leeds, Leeds, LS2 9JT, UK*

**py18ajs@leeds.ac.uk*

Auxetic materials have a negative Poisson's ratio and exhibit the peculiar property of an increasing thickness in a direction perpendicular to an applied strain. Auxetic materials have increased indentation resistance and energy absorption in comparison to non-auxetic materials [1], making them promising for a large range of potential applications, from sports equipment to automotive safety. Whilst an auxetic response is typically mediated by an increasing volume of macroscopic pores under strain, in 2018 an acrylate liquid crystal elastomer (LCE) was shown to display auxetic behaviour at the molecular level such that total volume is conserved [1].

The order in two similar auxetic LCEs consisting of the same base mesogenic and non-mesogenic monomers but a different proportion of crosslinker has been determined via polarised Raman spectroscopy (PRS). PRS allows for uniaxial order parameters, $\langle P_{200} \rangle$, $\langle P_{400} \rangle$, and the biaxial order parameters, $\langle P_{220} \rangle$, $\langle P_{420} \rangle$, $\langle P_{440} \rangle$, to be determined in addition to the director angle [3]. The LCEs were analysed as a function of nominal strain, ϵ , perpendicular to the initial director. The uniaxial order parameters for both the greater crosslinked and the lesser crosslinked materials show similar behaviour, with $\langle P_{200} \rangle$ reducing from initial unstrained values of $\langle P_{200} \rangle = 0.53 \pm 0.05$ and 0.60 ± 0.05 respectively to within error of zero at strains of $\epsilon \sim 1.0$. The strain at which zero order parameter occurs is a dark state under crossed polarisers and is immediately followed by a director rotation (a so-called mechanical Fréedericksz transition) [2, 3]. A detailed analysis indicates that both samples show biaxial behaviour from low strains [3]. Further, the order parameter data allows the orientational distribution functions to be determined as a function of strain.

Here, we contrast the similar order parameter behaviour seen for both LCEs with the rather different auxetic response of the two materials with strain. Both materials only exhibit a negative Poisson's ratio at strains larger than a specific threshold which are $\epsilon \sim 1.00 \pm 0.05$ for the greater crosslinked material and $\epsilon \sim 0.58 \pm 0.05$ for the lesser crosslinked material [2, 3]. We consider why the strain at which the mechanical Fréedericksz transition occurs is the same for the LCEs while the auxetic threshold is considerably different.

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Alignment of Chromonic Liquid Crystals

A.S. Alshammari*^a, T. Moorhouse, C. Jones, M. Nagaraj

^a *School of Physics and Astronomy, University of Leeds, Leeds LS2 9BW, United Kingdom*

* pyassa@leeds.ac.uk

The local control of anisotropic properties is necessary for a wide variety of new applications, including water-based electrical devices and biological sensors. Lyotropic chromonic liquid crystals (LCLCs), are an interesting type of material that, in most cases, are biocompatible and biodegradable [1]. These materials also offer uniaxial anisotropy through a director field. Lyotropic chromonic liquid crystals (LCLCs) are made up of molecules that self-assemble into elongated aggregates, which then form nematic or columnar LC phases depending on temperature and concentration [2]. Compared with thermotropic LCs, aligning lyotropic chromonic liquid crystal (LCLC) has proven difficult in the past. This has been related to the limited anchoring energy provided by traditional rubbing or coating techniques for stable LCLC alignment [1, 3].

In this work, we present a novel approach to chromonic liquid crystal alignment based on surface relief gratings (SRG) with the ultimate aim of obtaining accurate measurements of physical properties such as absorption anisotropy, birefringence, and order parameter and potentially high frequency permittivities. Our alignment technique is based on surface topography microstructures. Sunset Yellow (SSY) was used to demonstrate the alignment of a chromonic nematic phase. We compare the alignment of LCLCs using the traditional alignment techniques such as rubbed polyimide (PI) and Polyvinyl alcohol (PVA) with that obtained using the surface relief grating. We accomplish patternable planar alignment of Sunset Yellow and anticipate that our approach to director field control will lead to new possibilities for the fabrication of LC-based electronics and biological devices.

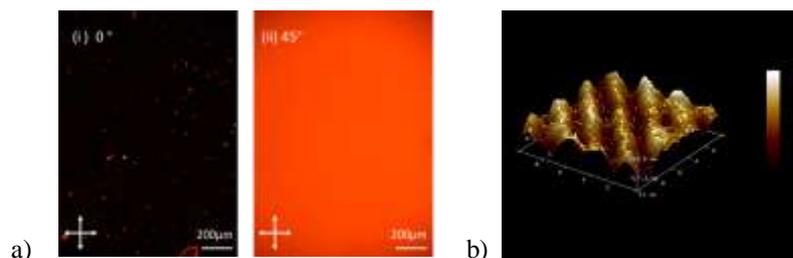


Figure 1. a) Polarized optical microscopy images of planar-aligned SSY sandwiched between two grating coated glass substrates. The dark image has an alignment under the crossed polarizers and the bright image has no alignment. b) AFM images of the SRG.

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* Author for Correspondence: pyassa@leeds.ac.uk

Liquid Crystal Materials for THz frequency adaptive optics

H. Godden^{*a}, A. Dunn, Z. Zhang, M. D. Horbury, A. D. Burnett, H. F. Gleeson, and A. Valavanis

Faculty of Engineering and Physical Sciences, University of Leeds, Leeds LS2 9JT, UK

[*elhig@leeds.ac.uk](mailto:elhig@leeds.ac.uk)

Liquid crystals (LCs) have a long history of being used in optical components, most notably in the visible spectrum where they have been well documented. Terahertz (THz) frequencies are the band of the electromagnetic (EM) spectrum between microwaves and infrared, often quoted as the frequencies from 0.3–10 THz (0.03–1 mm). THz radiation has seen much interest in the last few decades as sources have become increasingly more powerful and compact, underpinning a wide range of applications including atmospheric and space research, security, and biomedical sensing, owing to the unique “fingerprints” of many chemical species in the THz band [1].

One of the challenges in this field is the lack of commercial optical components, and even more so, adaptive optics (AOs). LCs have shown promise at THz frequencies with devices such as a phase-shifter being presented at 1.0 THz showing a greater than $\pi/2$ shift [2]. However, these studies have typically been limited to frequencies below the 2–5-THz range associated with high-powered THz quantum-cascade laser (QCL) sources. We have recently demonstrated power modulation of THz QCLs using LCs, showing substantial modulation depths of up to ~40% at 3.4 THz (Fig. 1) [3]. Due to the long wavelength of THz radiation, however, the LC devices are required to be much thicker than their counterparts for the visible spectrum. This makes it especially important to document and characterise LCs throughout the THz band to find optimal parameters in order to minimise the thickness of LC devices. In this presentation we demonstrate recent progress in the THz characterisation and analysis of LC materials, and the development of LC cells with THz transmissive window and electrode voltage materials.

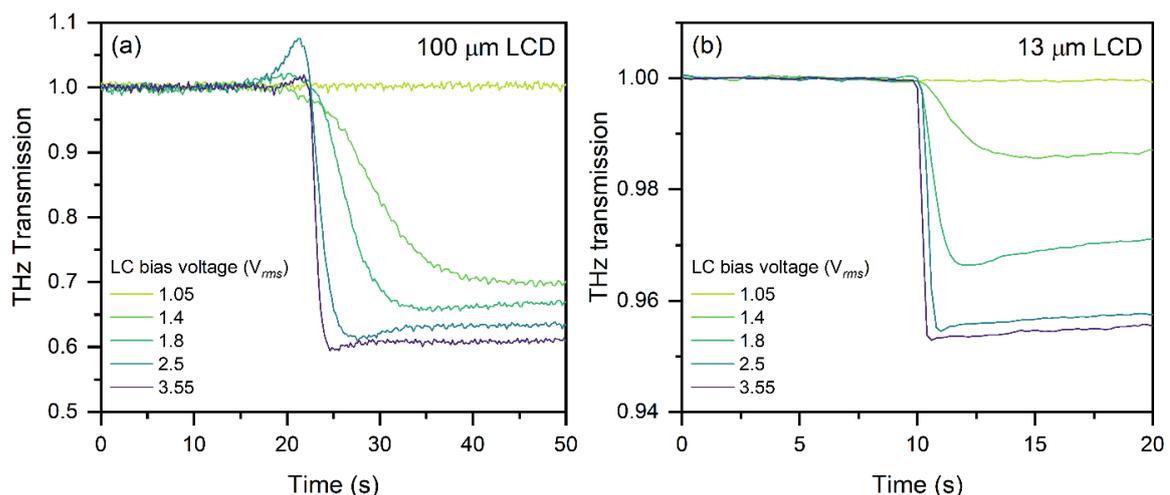


Fig 1. Transmission of linearly polarised 3.4 THz light when passing through the extraordinary axis of two LC cells with thicknesses of (a) 100 μm and (b) 13 μm for different bias voltages [3].

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Synthesis of Liquid Crystal Elastomers in Flow System

J. Xu^{*a}, R.J. Mandle^{a,b}, D.A. Mistry^a

^a School of Physics and Astronomy, University of Leeds, Leeds, LS2 9JT, UK

^b School of Chemistry, University of Leeds, Leeds, LS2 9JT, UK

*pyjx@leeds.ac.uk

Liquid crystal elastomers (LCEs) combine the properties related to liquid crystal mesophases and polymer networks. Compared to low molar mass liquid crystals, they have limited molecular mobility and less bulk fluidity. Due to their responsive deformation behaviours to external stimuli, LCEs are recognised as promising materials for developing soft robotics actuators [1].

The molecular weight and its distribution of LCE products are mainly affected by the synthesis methods, which in turn contribute to their structure-property relations [2]. LCEs are conventionally prepared in batch reactors in published research [3]. Batch processes generally lack control over reagent dosing and certain reaction parameters (e.g. temperature control, mixing), resulting in broad molecular weight distribution and poor consistency in scale-up processing for commercial products. Flow chemistry has emerged as an alternative strategy to solve these problems [4].

To our best knowledge, no research has been done on synthesising LCEs in flow systems. In this project, the synthesis of LCEs based on thiol-acrylate Michael addition polymerisation are performed in batch and flow processes with optimised reaction temperature and flow rates [5]. Here, solutions of monomers and catalysts (with precise concentrations) are continuously pumped through microfluidic tube reactors at fixed flow-rates. Taking advantages of large surface-to-volume ratio, flow process provides far more effective mass and heat transfer, suppressing hot spots formation, and thus enhances the reproducibility and scalability of the products.

Figure 1 shows a schematic overview of the batch process, our flow system, and the chemical structure of monomers employed. The results of size exclusion chromatography (SEC) prove that the LCE production technology is improved by flow process, which is essential for tailorable structure design and physical properties study of LCEs.

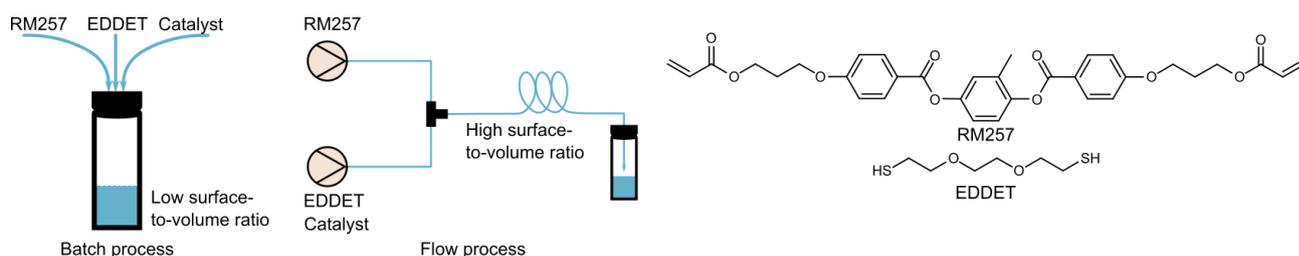


Figure 1. Reactor setups for batch and flow processes.

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Investigating how hairpin-like characteristics effect mechanical dissipation in liquid crystal elastomer networks

Meg Coleman*^a, P.D. Thornton^b, D.A. Mistry^a

^a *School of Physics and Astronomy, University of Leeds, Leeds, LS6 9JT, UK*

^b *School of Design, University of Leeds, Leeds, LS6 9JT, UK*

*py18mc@leeds.ac.uk

Personal protective equipment is required in many sporting and professional activities where injuries are likely. Current solutions to these scenarios include the use of expanding polystyrene and other materials to absorb impact energy, yet these are subject to failure under a variety of circumstances [1]. For this reason, all the shock absorbing materials currently available are single use. We require new materials that can withstand high impact energy without failure. This would enable more individuals to participate in activities such as cycling without the threat of injury, thus reducing the strain on the health service.

Liquid crystal elastomers (LCEs) are unique materials that combine rubber-like elasticity with the orientational order of liquid crystals. They are formed through the crosslinking of liquid crystal units with spacer units and provide a variety of characteristics including remarkable mechanical and dissipative properties [2]. It is currently hypothesised that LCEs can dissipate high amounts of energy due to the change in liquid crystal orientation upon shock. This hypothesis is currently only speculated: the evidence to prove it is flawed and there is an overall lack of fundamental understanding as to why these materials possess the desirable dissipative properties. To test the hypothesis, we plan to add 'kinks' and 'hairpin-like bends' into the LCE network by replacing a small percentage of the linear spacer units with permanently bent spacer units. This will create a static bend in the network. By mechanically testing these materials against those without hairpin bends, we can begin to assess the network characteristics that influence the amount of dissipation the LCE is capable of. This research has the potential to aid in optimising the dissipative characteristics seen in LCEs, which can then be used to benefit society.

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Interaction of Pf4 tactoids with bacteria and synthetic colloidal rods

Mariana de Oliveira Silva^a, Iago Grobas^a, **Yucen Han**^{*b}, Apala Majumdar^b, Lei Zhang^c, Abul Tarafder^d, Tanmay Bharat^d, Dirk Aarts^a

^a *Department of Chemistry, Physical and Theoretical Chemistry Laboratory, University of Oxford, United Kingdom*

^b *Department of Mathematics and Statistics, University of Strathclyde, United Kingdom*

^c *Beijing International Center for Mathematical Research, Peking University, China*

^d *Sir William Dunn School of Pathology, University of Oxford, Oxford OX1 3RE*

*yucen.han@strath.ac.uk

We investigated the interaction of tactoids [1] formed by a phase separating system of elongated virus particles and polymer with rod-like impurities. The elongated virus particles were Pf4, which when mixed with sodium alginate as polymer, phase separated into an isotropic phase in coexistence with a nematic phase of the virus particles [2]. The nematic phase appeared in the form of spindle shaped droplets called tactoids. We studied the interaction of this mixture with micrometer sized rods, which were either bacteria (or) or inert colloidal particles (made of SU8 or silica). Confocal laser scanning microscopy was used to examine the mixtures and four different dominant configurations were found, classified as no attachment, partial attachment of the rod to the tactoid, a “sandwich” state, where two tactoids interact with the same rod, and lastly encapsulation of the rods by the tactoids. We categorized the results in terms of surface properties and rod geometry (size and aspect ratio). To further elucidate this problem, we explored the system theoretically within a Ginzburg–Landau free energy. We obtained all the states seen empirically, and further noticed that the rod preferred to be close to the tip of the tactoid, probably due to the proximity of the defect to the one at tip of the tactoid, minimizing the energy of the system.

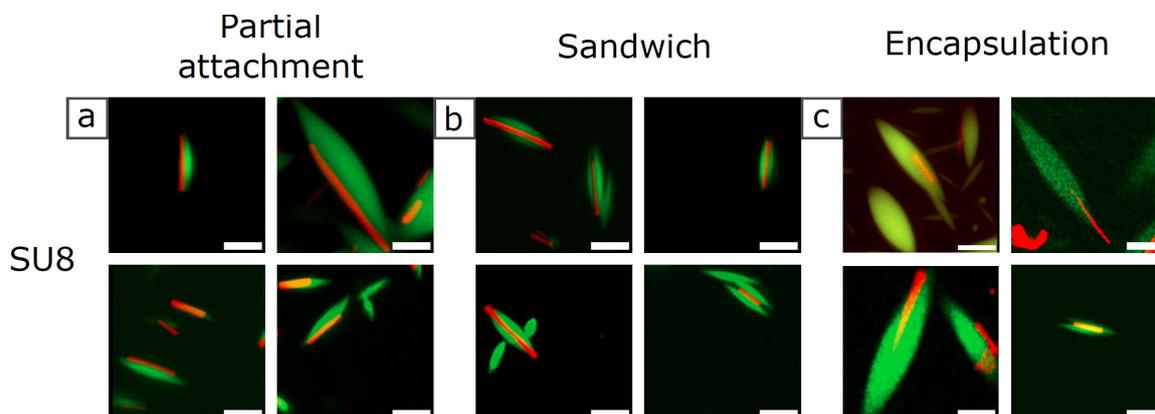


Figure 1: Configurations obtained for the synthetic rods. Confocal microscope images of SU8, in red, interacting with Pf4 tactoid, in green, (a) partial attachment, (b) sandwich, and (c) encapsulation.

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Optical and electrical properties characterisation of photovoltaic spatial-light modulators through cross-polarised intensity measurements

N. Brouckaert^{*a}, D. Bankova^a, O. Hovorka^a, T. Heiser^b, G. D'Alessandro^c and M. Kaczmarek^a

^a *School of Physics and Astronomy, Southampton SO17 1BJ, United Kingdom*

^b *ICube Research Institute, Université de Strasbourg, Strasbourg Cedex 2 67037, France*

^c *School of Mathematics, Southampton SO17 1BJ, United Kingdom*

*nb1f20@soton.ac.uk

Photovoltaic spatial-light modulators (PSLMs) are a self-powered version of liquid crystal devices (LCDs) that use an organic photovoltaic unit (PVU) as an integrated power source [1]. This technology allows a transition from a transparent to an opaque state when exposed to specific wavelengths. This is a versatile technology where both the absorbed wavelength and the modulated one can be tuned to adapt to any needs.

In this study, we present a method to fully characterise the cell photovoltaic properties such as photovoltage and photoconductivity, as well as liquid crystal critical properties, such as elastic constants, pretilt or anchoring energy, using non-invasive cross-polarised intensity (CPI) measurements. This technic makes it possible to follow the aging of the photoconversion despite the lack of direct electrical contacts. An extension of the method that allows a mapping of all these properties over the PSLM active area will be described [2].

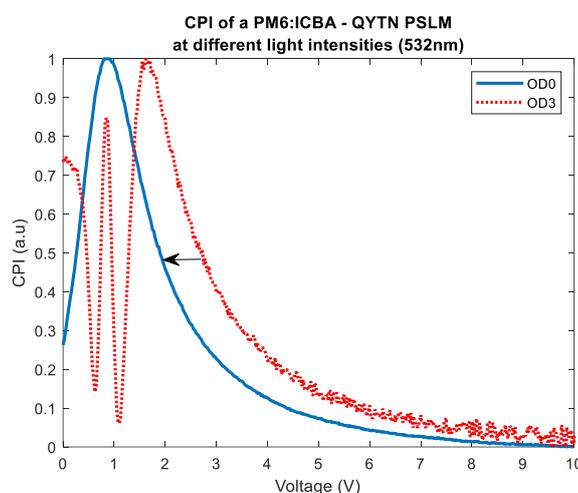


Figure 1. CPI of a PSLM at low (OD3) and high (OD0) light intensities (532nm). The photovoltaic unit (PM6:ICBA) is generating a photovoltage of 687mV when exposed to light (OD0). This additional voltage is contributing to the liquid crystal (QYTN) voltage needs to be reoriented, causing a shift of the CPI.

The authors would like to acknowledge Sadiara Fall and Yaochen Lin, along with the Icube laboratory, for their help to prepare the photovoltaic units.

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Structure Prediction and Self-Assembly of Multipolar Nematic Colloids

J.A. Morris^a, D. Chakrabarti^a

^a *School of Chemistry, University of Birmingham, Edgbaston, Birmingham, UK*

*jam534@student.bham.ac.uk; d.chakrabarti@bham.ac.uk

Nematic colloids are hybrid soft matter systems which have received much attention for their highly anisotropic, elasticity mediated pair-interactions which can facilitate a variety of self-assembled composite materials, as well as for their tunability in response to relatively weak external stimuli [1]. Colloidal inclusions induce energetically costly distortions in the nematic alignment, which yield spatial distortions in $\mathbf{n}(\mathbf{r})$, analogous to multipoles such as dipoles and quadrupoles found in electrostatics. The systems tend to reduce free energy via the sharing of these distortions, giving rise to effective anisotropic interactions between pairs of nematic colloids, which can be described by multipole expansion. Depending on the exact nature of the inclusions (including particle size and boundary conditions) the leading order multipole of the nematic colloid can be tailored, with dipoles, quadrupoles and other higher order multipoles being observed experimentally [2]. Under the multipolar expansion approximation, one can determine an effective pair potential to model the elastic interactions between pairs of colloidal particles [3], which have been used extensively in fitting with experimental data to model interactions at the pair level. However thus far there has been limited research in using this effective interaction to study many-body effects. In this context, we develop a computational framework for crystal structure prediction for multipolar nematic colloids interacting, using the basin-hopping algorithm. We explore the crystal lattice energy landscape in order to find the global and other low-lying minima available to a given multipolar colloidal building block in the presence of screened electrostatic repulsion. Additionally, we investigate how the crystal energy landscape is sampled under thermal conditions using Monte Carlo simulations to predict the self-assembly behaviour of the multipolar nematic colloids.

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Instabilities in active nematic liquid crystals subject to an applied orienting field

Ijupatil Joseph K., Nigel J. Mottram, Katarzyna N. Kowal, Joseph R. L. Cousins
School of Mathematics and Statistics, University of Glasgow, UK
Email: i.joseph.1@research.gla.ac.uk

Motivated by applications of active liquid crystals in the design of sensors and various biological processes, we present a theoretical and computational study involving the mathematical modelling of active nematics using an adapted form of the Ericksen-Leslie equations. We consider the effect of a combination of activity and orienting field on active nematics with a director confined between two parallel plates in a 1D geometry, subject to either planar or homeotropic anchoring conditions and no-slip conditions on the boundaries of the channel [1, 2]. We first solve the system analytically by linearising around a uniform director that is aligned with the anchoring conditions. The behaviour is characterised by a critical parameter, below which the system exhibits a no-flow state with no director distortion, which is unstable for contractile active agents and stable for extensile active agents. For contractile active agents, the director is distorted whenever the activity is above the critical activity. In the presence of an orienting field, the system becomes stable for extensile active agents whenever the behaviour is characterised by a critical activity, and the orienting field is below a critical value, and unstable otherwise.

Our results show that the system eventually exhibits one of three solution states: symmetric distorted, antisymmetric distorted, and uniform states. The uniform state corresponds to a uniform alignment of the director normal parallel to the boundaries of the channel. For field strengths greater than a critical value, the uniform state is replaced by the symmetric solution. For antisymmetric solutions, there is a reorientation in the middle of the layer with high elastic energy. Interestingly, the critical activity changes as we increase the magnitude of the orienting field. For low activity parameter values, the orienting field dictates the behaviour and the director angle in the middle of the layer prefers to align along the shear gradient. However, increasing the activity decreases the director angle at the middle of the layer, indicating that activity is reducing the distortion and eventually overriding the field effect, giving rise to the antisymmetric solution. Our results have potential applications for designing sensors and in improving our understanding of many biological processes such as biofilm formation and morphogenesis.

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Triphenoxazoles - a new class of Photoconducting Liquid Crystalline materials for organic electronic applications

Karolis Virzbickas,^{*a} Owen M. Jones,^a Michael S. Butlin,^a Jon A. Preece,^a Alex P.G. Robinson^b

^b School of Chemistry, University of Birmingham, Edgbaston, Birmingham, B15 2TT (UK)

^a School of Chemical Engineering, University of Birmingham, Edgbaston, Birmingham, B15 2TT (UK)

*Corresponding author: E-mail: v.karolis@bham.ac.uk

We develop triphenoxazole based novel broad-spectrum emitters designed for solution processed organic light emitting devices (OLEDs). Triphenoxazoles are a novel family of homologous compounds.¹ These materials exhibit a diverse array of material properties, from chemically tunable Stokes shifts, with emission from 400 nm to 650 nm, photoconduction, photovoltaic, and electroluminescence effects, as well as displaying ordered hexagonal columnar mesophase. Physical properties such as photoconduction are modulated through the control of the moiety attached to the C-2 of the oxazole unit. The triphenoxazole derivative with aromatic groups exhibits photoconductivity up to $\sim 1 \times 10^{-8}$ S/cm, the largest $\sigma_{\text{photo}}/\sigma_{\text{dark}}$ ratio of $\sim 1.71 \times 10^3$, which is two orders of magnitude higher than that of alkoxytriphenylene, with charge carrier mobilities of $\sim 1 \times 10^{-3}$ cm²/Vs.

Blue, green, and orange color OLEDs were fabricated with triphenoxazoles as an emissive layer in Figure 1. Hence, triphenoxazoles provide a platform for the design of new organic broad-spectrum emitters for OLED lighting applications.

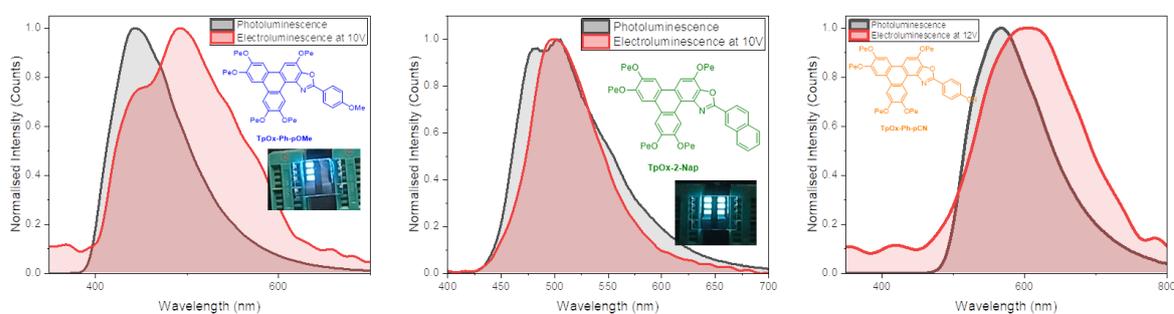


Figure 1 shows electroluminescence spectra of OLED device in red and photoluminescence spectra in black of (a) TpOx-Ph-pOMe, (b) TpOx-2-Nap and (c) TpOx-Ph-pCN.

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Effect of Anisotropic Nanoparticles on the Dielectric Susceptibility of Nematic Nano-Composites: A Molecular Theory

M.A.Osipov*^a, A.S.Mererkalov^b, A.A.Ezhov^c

^a *Department of Mathematics and Statistics, University of Strathclyde, Glasgow, UK*

^b *Topchiev Institute of Petrochemical Synthesis, Russian Academy of Sciences, Moscow, Russia*

^c *Faculty of Physics, Lomonosov Moscow State University, Moscow, Russia*

*m.osipov@strath.ac.uk

The effect of rod-like nanoparticles on the high-frequency dielectric susceptibility of the nematic nano-composites has been investigated in the framework of a molecular theory. Analytical expressions for the components of the effective polarizability of a rod-like nanoparticle in the nematic host have been obtained and used in the calculations of the dielectric susceptibility of the composites as functions of the nanoparticle volume fraction [1]. Numerical calculations of the susceptibility have been undertaken using the nematic liquid crystal 5CB as a host doped with either gold or silver particles for different values of the concentration of nanoparticles. It has been shown that the rod-like nanoparticles have a much stronger effect on the components of the dielectric susceptibility of the nano-composites in comparison with spherical nano-particles [2] including, in particular, the one with gold nanoparticles in the vicinity of the plasmon resonance. The main conclusion is that at sufficiently large concentration of nanoparticles, the anisotropy of the dielectric susceptibility of the nano-composites may even change the sign with an increasing concentration which may be important for various applications.

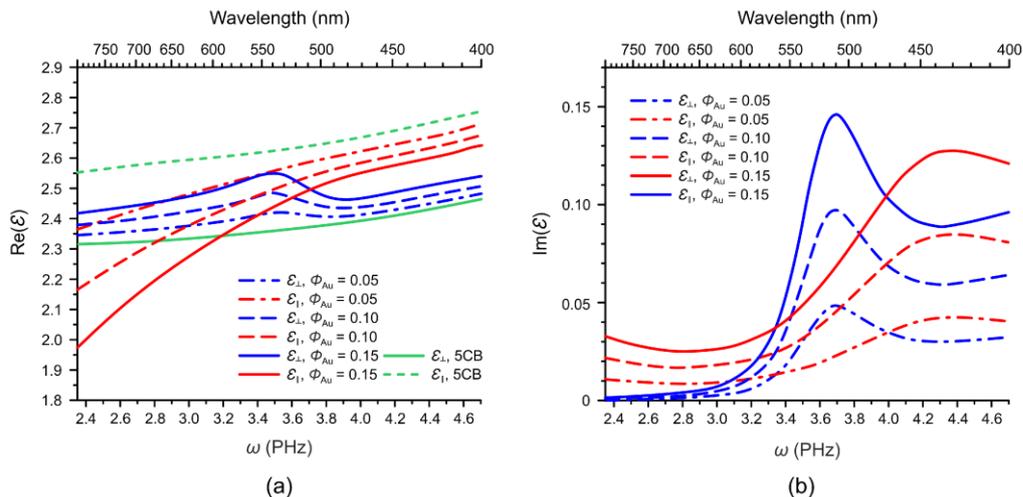


Figure 1. Real (a) and imaginary (b) parts of the transverse and longitudinal components of the high-frequency dielectric susceptibility of the 5CB nematic nano-composites for different values of the volume fractions of AuNPs.

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Microscopic viscosity measurements of liquid crystal phases using ferrofluid droplets

Varun Chandrasekar, Ingo Dierking, Jian Ren Lu

Department of Physics and Astronomy, University of Manchester, Manchester, M13 9PL, UK
varun.chandrasekar@postgrad.manchester.ac.uk

Many liquid-crystalline (LC) phases are exhibited in nature and a decent amount of them have a wide variety of applications. The properties of these LC phases can be studied in terms of their respective kinematic viscosities. Here, we microscopically measure the viscosities of certain LC phases that are not too viscous. To measure these, a ferrofluid consisting of chemically treated magnetite stably dispersed in a Newtonian carrier fluid which is immiscible with the LCs is used. The ferrofluid is dispersed in the LC with spherical microscopic ferrofluid droplets obtained. By use of a neodymium bar magnet the spherical ferrofluid droplets in the liquid crystal can be moved. The anisotropic viscosities of different LC phases are determined using a modified version of Stokes' law.^[1] The viscosities of various thermotropic, lyotropic and colloidal LCs, along with their temperature and concentration dependence, are provided in this study.

To initially verify this measurement method, the anisotropic viscosities of thermotropic nematic 5CB (4-Cyano-4'-pentylbiphenyl) are measured and compared with reported values ^[2]. Similarly, the viscosities of 8CB (4-Cyano-4'-octylbiphenyl) are measured across the smectic A-nematic transition temperature range and the measured values are verified with the reported values ^[2]. The viscosities of cholesteric 5CB + S811 (S-(+)-2-Octyl 4-(4-hexyloxybenzoyloxy) benzoate) mixtures were studied as the pitch changes over the order of magnitude of the size of the probe droplet, producing a variable anisotropy behaviour. In terms of lyotropic LCs, the viscosities of amphiphilic CTAB (Cetrimonium bromide) and chromonic Sunset Yellow FCF are measured, and the concentration dependence of the respective viscosities are provided. In terms of colloidal LCs, the anisotropic viscosities of cholesteric cellulose nanocrystals (CNCs) are measured as a function of concentration through the two-phase region. Additionally, the anisotropic viscosities of colloidal nematic graphene oxide (GO) are measured and the concentration dependence is studied for two separate colloidal arrangements.

LC-Ferrofluid emulsions can potentially be used in many applications and the next step for this work is to create a synthetic structure which mimics a magnetotactic bacterium (MTB)
^[1].

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