BLCS

The British Liquid Crystal Society

The British Liquid Crystal Society
40th Annual Meeting
2026

Tue 14th - Thu 16th of April 2026

University of Warwick

School of Engineering and Physics Department

Physics Lecture Theatre and the Science Concourse

Abstract Booklet

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Contents

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Liquid Crystals

The 2026 BLCS Annual Meeting

DAY 1: TUESDAY 14 APRIL @ THE PHYSICS LECTURE THEATRE (PLT)

9:30-10:00	Welcome coffee
10:00-11:00	**Plenary: Nematic, Smectic and Cholesteric Liquid Crystal Droplets - Exotic Defects, Lunes and Focal Conic Domains for New-Age Applications.** Apala Majumdar FRSE, FIMA, University of Manchester, UK
11:00-11:40	coffee break
11:40-12:00	**Columnar Ordering in Triphenoxazoles: Molecular Simulations Insights into a New Class of Fluorescent Discotic Liquid Crystals** Dwaipayan Chakrabarti, University of Birmingham, UK
12:00-12:20	**The Homogenised Energies for Suspensions of Colloidal Nanoparticles in Nematic/Cholesteric Liquid Crystals** Fatimah Almutari, University of Strathclyde, UK
12:20-12:40	**Subcritical Flow Transitions in Active Nematics** Alexander Houston, University of Glasgow, UK
12:40-12:50	Nigel Balmforth, **Taylor and Francis**
13:00-14:00	Lunch, Radcliffe
14:00-14:20	**Structuring Liquid Crystals under Confinement Conditions by Neutron Scattering** Oleksandr Tomchuk, ISIS Neutron and Muon Source, UKRI, UK
14:20-14:40	**Measurements of the Air/LC Interface Tilt Angle in Unusual Nematic Liquid Crystal Systems** Abigail Bond, University of Leeds, UK
14:40-15:00	**Thermal resolution limit for thermochromic liquid crystals sensors for sensing ultrasound** Martha Turvey, University of Warwick, UK
15:00-15:40	coffee break
15:40-16:20	poster flash talks
16:20-18:00	**Poster Presentations** and welcome reception Science Concourse

DAY 2: WEDNESDAY 15 APRIL @THE PHYSICS LECTURE THEATRE (PLT)

10:00-11:00	**Plenary: Exploring Colloidal Liquid Crystals Through Filamentous Phage Model Systems** Eric Grelet, Centre de Recherche Paul-Pascal, CNRS & University of Bordeaux, France
11:00-11:40	coffee break
11:40-12:00	**Full vectorial-field sensing based on inkjet-printed LC droplets** Jinge Guo, University of Oxford, UK
12:00-12:20	**Blue Phases on PCB: Unlocking fast phase modulation** Oana Niculescu, University of Cambridge, UK
12:20-12:40	**Electrically Switchable vari-focal Continuous Phase Liquid Crystal Fresnel Zone Plate** Zhiyu Xu, University of Oxford, UK
12:40-13:00	**Adaptive Coherence Control for Holographic Measurement Systems using a Liquid Crystal Coherence Modulator** Tianxin Wang, University of Oxford, UK
13:00-14:00	Lunch, Radcliffe
14:00-15:20	Prize giving and Young Scientist lecture
15:20-16:00	coffee break
16:00-16:20	**Design Principles of Fluid Molecular Ferroelectrics** Calum J. Gibb, University of Leeds, UK
16:20-16:40	**Modulated Anti-Ferroelectric Smectic Phases with Orthogonal and Tilted Structures** Jordan Hobbs, University of Leeds, UK
16:40-17:00	**Computational approach for rapid screening for ferroelectric order in nematogens** Mark Wilson, Durham University, UK
17:00-17:20	**Dipoles, boundary conditions, and the ferroelectric nematic phase** Saud Al-Qabandi, University of Manchester, UK
17:20-18:00	AGM
19:00-21:30	Conference 40th dinner and Hilsum medal talk

DAY 3: THURSDAY 16 APRIL @ THE PHYSICS LECTURE THEATRE (PLT)

10:00-10:40	**Invited Speaker:** **Frustrated Smectic Liquid Crystal Elastomers as Multifunctional Mechanical Metamaterials** Stuart Berrow, University of Leeds, UK
10:40-11:00	**Mechanically reconfigurable auxetic metamaterials based on shape memory effect** Zhenming Wang, University of Leeds, UK
11:00-11:40	coffee break
11:40-12:00	**Diverse helical structures made of achiral mesogenic dimers** Abigail Pearson, University of Aberdeen, UK
12:00-12:20	**Synthesis and characterisation of liquid crystals bearing a sustainable novel uracil derived headgroup** William Ogle, University of Leeds, UK
12:20-12:40	**Structure-Property Relationships of Polar Mesogens Containing Sulfur** Ewan Cruickshank, Robert Gordon University, UK
12:40-13:00	student prizes and closing remarks
13:00-13:20	Lunch, packed
13:20-14:00	BLCS committee meeting

LIST OF POSTERS: TUESDAY 14 APRIL (16:20 - 18:00)

Poster No.	Presenter	Organisation	Title
P1	Cameron Smith	University of Warwick	Chevron Instabilities in Active Smectic Liquid Crystals
P2	Sarangi Krishna	Sheffield Hallam University	Towards the mesoscopic simulations of Liquid Crystal Elastomers
P3	Thuriya Al Hinai	University of Strathclyde	Stability of Nematic Equilibria in Isosceles Triangular Domains
P4	Sam Bainbridge	University of Manchester	Nematic Liquid Crystal Configurations in Triangular Confinement
P5	Harry J. Godden	University of Leeds	Control of a Dual-Frequency Liquid Crystal Variable Attenuator for the Power Stabilisation of a Terahertz Quantum-Cascade Laser
P6	Aleksandra Symanovic	Ruđer Bošković Institute, Chroatia	From Bpiii To Helix Inversion: Mesomorphic Behaviour And Chirality Transfer In Chiral Mesogenic Dimers
P7	Zhenming Wang	University of Leeds	Multidimensional Multilevel Information Storage and Encryption in Auxetic Liquid Crystal Elastomers
P8	Shona Ramsay	University of Aberdeen	Synthesis and Characterisation of Fluorinated Ferroelectric Nematogens
P9	Martha Turvey	University of Warwick	Acoustic control of soft matter-based composites

Key	Topic
🟨	theory and simulation
⬛	elastomers
⬜	applications
🟦	experiment
🟪	ferroelectrics
🟧	synthesis

Nematic, Smectic and Cholesteric Liquid Crystal Droplets - Exotic Defects, Lunes and Focal Conic Domains for New-Age Applications

Apala Majumdar FRSE, FIMA
University of Manchester, UK

We review continuum Landau-de Gennes-type theories for the nematic, smectic and cholesteric liquid crystal phases in confined geometries. We introduce the essential mathematical frameworks and then apply these methods to model nematic, smectic and cholesteric liquid crystal droplets respectively. We illustrate how the different types of liquid crystal ordering manifest in different types of liquid crystal profiles within the droplets, including the different types of defect structures stabilised by nematic, smectic and cholesteric order respectively. We compare our modelling results with experiments on liquid crystal droplets, and discuss their applications to counterfeiting, photonics and microfluidics. All collaborations will be acknowledged during the talk.

Columnar Ordering in Triphenoxazoles: Molecular Simulation Insights into a New Class of Fluorescent Discotic Liquid Crystals

Wilson, Mark R.[1]; Bupathy, Arunkumar[2,3]; Chakrabarti, Dwaipayan[2]

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[2] *School of Chemistry, University of Birmingham, Birmingham B15 2TT, UK, d.chakrabarti@bham.ac.uk*

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Atomistic simulations are becoming a powerful tool for understanding molecular order in complex liquid crystalline phases.[1-3] Such simulations are able to rationalize how changes in molecular structure control the close packing of molecules, and how preferred molecular interactions can stabilize (or destablize) liquid crystal mesophases. We perform atomistic simulations of representative mesogens from a class of newly synthesized fluorescent discotic liquid crystals. We demonstrate the spontaneous emergence of the columnar ordering, when cooled from the isotropic phase in simulations that extend into the μs regime. We characterise the columnar order and and its growth across the phase transition.

Our simulations show the formation of molecular stacks in the pretransition region and suggest that the transition into the columnar phase is achieved by the coalignment of these stacks. We analyse the structure of the columnar phase as well as the local arrangements of the molecules within the columns and discuss their implications for potential applications of this exciting class of compounds.

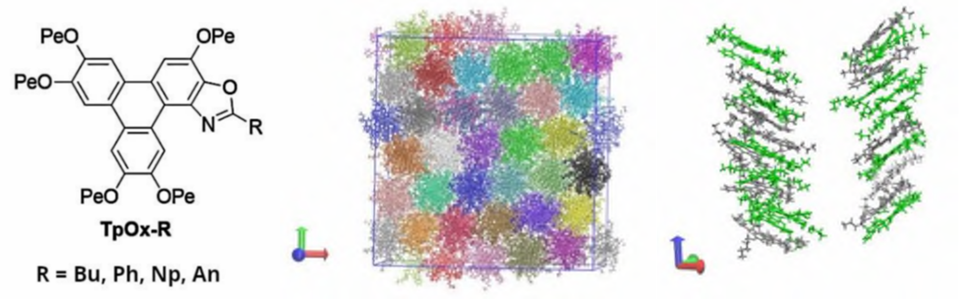

Figure 1: Left, chemical structures of the TpOx series; middle, simulation snapshot showing the ordering of columns in the columnar phase of TpOx-Ph; right, tilting of molecular cores in neighbouring columns in the columnar phase of TpOx-Ph.

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The Homogenised Energies for Suspensions of Colloidal Nanoparticles in Nematic/Cholesteric Liquid Crystals

Fatimah Almutari

We study the effects of colloidal nanoparticles (NPs) in liquid crystal samples in the dilute limit, in a Landau–de Gennes theoretical framework [1]. The effects of the suspended NPs are captured by a homogenized energy, as outlined in [2]. For spatially homogeneous samples, we explicitly compute the critical points and minimizers of the modified Landau–de Gennes energy and show that the presence of NP eliminates the first-order isotropic-nematic phase transition, stabilises elusive biaxial phases over some temperature ranges and that the symmetry of the NP boundary conditions or surface treatments dictates the bulk equilibrium phase at high temperatures. These biaxial solutions arise from the presence of nanoparticles and do not occur in the pure cholesteric or nematic phase. The homogenized energy sheds light into how the shape and anchoring conditions of the colloidal nanoparticles can be used to tune the physical properties of the composite material, i.e., the phase transition temperatures and the bulk properties. We conclude with some investigations of confinement effects on such composite systems and how the suspended colloidal nanoparticles can affect experimentally observable textures in benchmark geometries.

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Subcritical Flow Transitions in Active Nematics

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Active nematics model a wide range of living systems, including cells layers and bacteria [1]. One of the quintessential features of active nematics is that, when confined to a channel, they will transition to a flowing state once their activity exceeds a critical value [2]. Since its discovery over twenty years ago, this flow transition has been taken to be supercritical, associated with continuous growth in an unstable director mode. However, by applying a non-linear analysis we find that the transition can often be subcritical, associated with a discontinuous jump at the critical activity. We determine the regions of parameter space for which a subcritical transition occurs for both odd and even symmetry director modes, as shown in Figure 1. In addition to pronounced differences for the two mode types, we find distinct mechanisms driving subcriticality in different regions of parameter space, namely active stresses when the flow-alignment parameter is small and elastic stresses when it is large. Our work extends recent results on active nematic transitions [3] and indicates that the non-linear dynamics of confined active nematics leads to a richer phenomenology than previously thought.

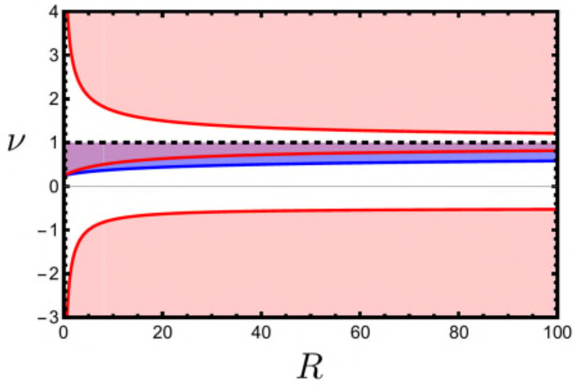

Figure 1: The regions of subcriticality as a function of flow alignment parameter, ν, and the ratio of rotational to shear viscosity, R. The different colours indicate the mode that exhibits a subcritical transition in that region: red (odd mode), blue (even mode) and purple (both).

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Structuring Liquid Crystals under Confinement Conditions by Neutron Scattering

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[1] ISIS Neutron and Muon Source, UK Research and Innovation, UK

[2] Institute of Nuclear Physics, Polish Academy of Sciences, Poland

Liquid crystals confined to restricted geometries display behaviours that differ profoundly from their bulk counterparts, as spatial limitations at the nanometre scale alter both molecular ordering and collective dynamics. Investigating these effects is essential not only for advancing the fundamental understanding of soft condensed matter under confinement, but also for informing the design of functional materials relevant to modern optoelectronic technologies. Confinement may occur in several distinct forms. In one-dimensional confinement, typical of thin-film geometries, liquid crystals are restricted along a single axis, making neutron reflectometry a particularly powerful tool for resolving interfacial structure, layering, and anchoring effects with sub-nanometre precision. Two-dimensional confinement arises in systems such as core-shell liquid-crystal/polymer fibres or liquid crystals imbibed into cylindrical nanoporous channels, where curvature and surface interactions strongly influence orientational order. Fully three-dimensional confinement is realised in nano- or micro-sized liquid crystal droplets dispersed within a polymer matrix, where both shape and interfacial topology play a decisive role. In the latter two cases, small-angle neutron scattering provides direct access to mesoscale morphology and spatial correlations. Overall, neutron scattering techniques offer uniquely detailed structural information on confined liquid crystals, enabling the characterisation of buried interfaces at the nanoscale.

This paper presents recent results of neutron studies of partially fluorinated terphenyl liquid crystals [1], demonstrating the potential of scattering methods in structural diagnostics due to the high penetrating power of neutron radiation.

[1] Tomchuk O., Drzewicz A., Len A., Ryukhtin V. J. Mol. Liq. 439 (2025) 128895.

Measurements of the Air/LC Interface Tilt Angle in Unusual Nematic Liquid Crystal Systems

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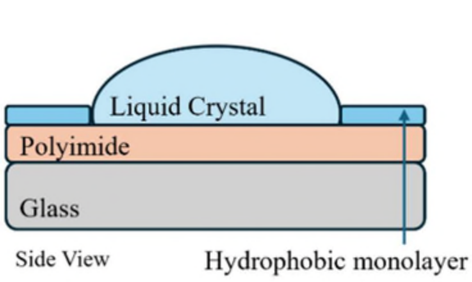
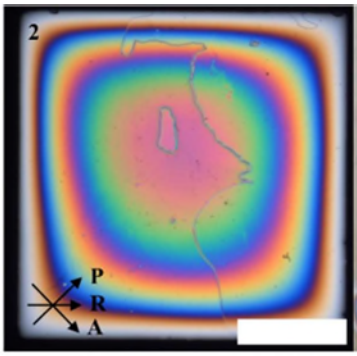
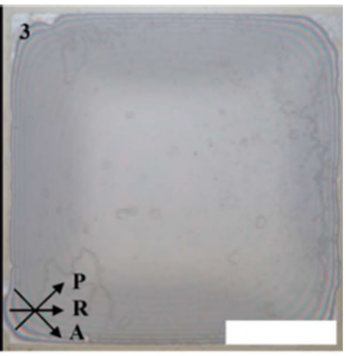
The liquid crystal (LC) director at bounding interfaces is key in the design of LC devices, however the anchoring is often labelled generally as homeotropic, tilted or planar without an exact director tilt angle. The air/LC interface anchoring is particularly important for LC-based sensing devices that rely on a change in anchoring on addition of an analyte, imaged under polarised optical microscopy[1]. Previous work[2] described a potential LC-based sensing device based on the nematic LC (NLC) E7, confined on a solid substrate with a chemically patterned 6 x 6mm square and a free air/NLC interface (Fig. 1). The choice of LC in such a system is important to ensure an air/NLC interface tilt angle that can provide a large optical contrast on addition of a range of analytes.

A facile method to measure the exact air/LC interface angle will be described using the NLC MLC 7023 confined in a 6 x 6mm chemically patterned square (Fig. 2). This mixture is chosen as it has been reported that the air/LC interface is not homeotropic[3]. It will be shown that MLC 7023 has an air/LC interface tilt angle of 84 ° and therefore should demonstrate greater optical contrast for both homeotropically- and planar- aligning analytes than E7 which aligns homeotropically. The method used to deduce the tilt angle in MLC 7023 will then be used to describe the behaviour of the nematic phase of ferroelectric nematic liquid crystal confined in a 6 x 6mm square (Fig. 3). On cooling through the nematic phase there is a plateau region in the effective birefringence, which we relate to a tilt angle between 89 ° -90 ° for 9.3 ° C–29.8 ° C below T_{NI} (Fig. 4) to 75 ° ~32 ° C below T_{NI}.

1







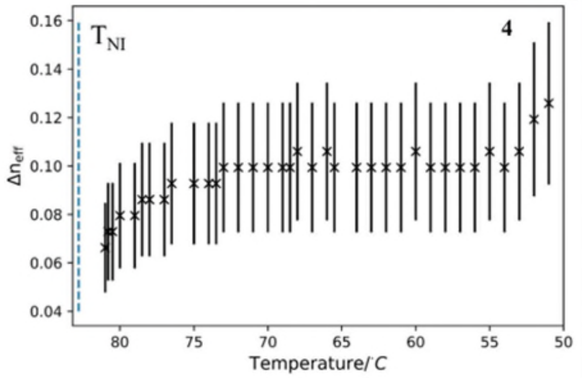


Fig.1: Schematic of the confinement of LC in a square delineated by a hydrophobic monolayer on a polyimide layer with a free air/LC interface. Fig. 2: Polarised images of MLC 7023 and Fig. 3: ferroelectric nematic liquid crystal confined in 6 x 6mm squares with heights of 42µm and 80µm, respectively. P, A and R are the relative polariser, analyser and rubbing directions. The scale bars are 2mm. Fig 4: Effective birefringence of the nematic phase of the confined ferroelectric nematic liquid crystal droplet.

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Thermal resolution limit for thermochromic liquid crystals sensors for sensing ultrasound

Martha Turvey[1], Oksana Trushkevych[1], Victor Reshetnyak[1], Rachel S Edwards[2]
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[2] *Department of Physics, University of Warwick*

Ultrasonic field visualisation is important for non-destructive testing applications, through finding and monitoring defects in components. Standard methods, such as laser vibrometry, involve scanning point-by-point across the surface to build up a map which offers high precision but can be time consuming and involves high cost equipment. Instead, thermochromic liquid crystal (TLC) sensors can be used to map ultrasound intensity across the surface of a sample[1,2]. Ultrasound absorbed within the sensor generates heat, which changes the pitch of chiral nematic LC inside thus altering the wavelength of reflected light. Figure 1(a) shows a photo of the sensor visualising the resonant field produced by an 18 mm diameter flexural transducer at 320 kHz. Temperature maps of the surface, comparable to ultrasonic intensity, can be extracted from image analysis of optical photographs of the sensor[3], as shown in figure 1(b). This temperature corresponds to several factors including the displacement, environment, and thermal conductivity of the sample.

The resolution limitations of the sensor have been investigated through modelling and experiments, by considering sensor thickness and thermal diffusion effects. Increasing thickness improves the sensitivity of the sensor, but reduces resolution. An initial resolution limit of the sensor between 0.35±0.02 mm and 0.51±0.09 mm has been determined through comparison of TLC, interferometry, and model data extracted from patterns produced by resonant transducers, demonstrating sub-millimetre resolution. An initial thermal model of the transducer has also been produced to obtain a more precise resolution limit for the sensor, with the results showing some of the expected thermal diffusion effects, but not yet matching the experimental results. Further work is being conducted to match the model to experimental results.

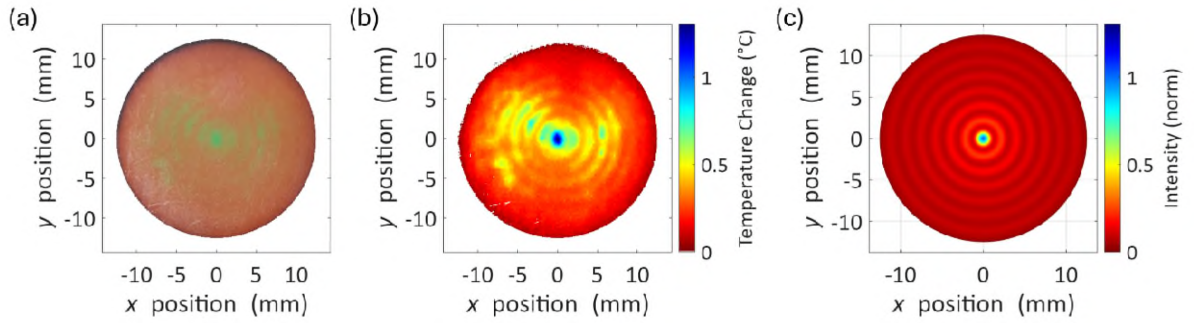

Figure 1. (a) Photo of TLC sensor visualising a resonant mode at 320kHz on an 25mm diameter transducer, (b) the temperature map extracted from the photo using image processing, and (c) the thermal model of the same mode.

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Exploring Colloidal Liquid Crystals Through Filamentous Phage Model Systems

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Filamentous bacteriophages, notably fd and M13, constitute a well-established model system for rod-like colloids in soft condensed matter, owing to their exceptional monodispersity in size and tunable interparticle interactions [1,2]. These features give rise to a rich phase behavior, including a wide variety of colloidal liquid crystalline states [3]. In this talk, we will present recent advances in the exploration of the phase behavior of such viral suspensions, with a particular emphasis on direct single-particle-level visualization and tracking to quantify the dynamics across the different mesophases [4,5].

We will discuss how confinement and topological defects influence the emergence and propagation of chirality from the particle scale to supramolecular liquid crystalline structures [6]. In particular, we will show that self-assembly into the cholesteric phase arises from the interplay between three key chirality amplification mechanisms, which have been identified and will be analysed discussed quantitatively [7].

We will then turn to strategies for regioselective functionalization of filamentous phages, enabling the formation of hybrid and more complex colloidal building blocks, such as star-like structures [8,9].

Overall, our work highlights the versatility of filamentous phage systems as model colloids for investigating liquid crystalline order, while opening perspectives for designing complex, functional materials based on bio-derived anisotropic particles.

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Full vectorial-field sensing based on inkjet-printed LC droplets

Jinge Guo[1] , Xuke Qiu[1] , Runchen Zhang[1] , Qihao Han[1] , Waqas Kamal[1] , Steve Elston[1] , Stephen Morris[1] , Chao He[1]

[1] *Department of Engineering Science, University of Oxford, UK*

We propose a multifunctional optical sensing platform based on inkjet-printed nematic liquid crystal (LC) droplets. These droplets exhibit voltage-dependent spatially-varying birefringence profiles governed by the anchoring conditions imposed by the droplet and surface properties, which we validate through both polarizing optical microscopy and numerical simulations.

We arrange the printed droplets in a 2-dimensional array to realize a division-of-wavefront scheme, enabling simultaneous measurement of the spatially resolved polarization and phase of light. The system combines Stokes polarimetry with a Shack–Hartmann-inspired method for wavefront sensing, and achieves single-shot polarization vector mapping without the need for mechanical scanning or polarizers. Moreover, red-green-blue imaging provides dual-wavelength capability through spectral separation.

This work demonstrates an integrated strategy for real-time, compact, and scalable optical diagnostics. By exploiting the remarkable optical anisotropy of printed nematic LC droplets, our platform paves the way toward full-field vectorial sensing across diverse photonic applications.

Blue Phases on PCB: Unlocking fast phase modulation

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The use of liquid crystalline materials in phase modulation has spanned applications from the infotainment industry (primarily through their use in Augmented Reality, holography, and displays), the automotive (with the growing use of head-up displays in cars), communications (holographic optical switching) and beyond into photonics for medical and scientific use (adaptive optics for ophthalmology and microscopy, pulse shaping, and optical filtering) [1]. Multi-level phase modulation is still commercially done with nematic Liquid Crystals as the primary medium.

This work provides an alternative solution, by using Polymer Stabilised Blue Phase (BP) Liquid Crystals instead, which comes with the benefits of polarisation insensitivity and submillisecond response times, while avoiding the use of alignment layers, simplifying device construction [2]. Furthermore, with these phase modulators, the range of applicability can be extended to long-range communications and astronomical adaptive optics, meeting the much higher switching rate required [3].

In the first part of this paper, the single pixel response of a BP device is verified to meet the expected performance. It is found to have a rise and fall time of t_{rise} =130 μs and t_{fall} = 125 μs, respectively. It achieves a phase modulation of 1.23 radians, corresponding to 0.39π, at an applied field of 7.73 V/μm in a transmissive topology.

For the second half, Blue Phases are grown directly on a Printed Circuit Board (PCB). These were specifically designed to apply Zernike modes, which are orthogonal modes describing wavefront deformations. A tip/tilt mode is successfully applied with a root mean square of the wavefront of 76.05 radians across a 1 cm x 1 cm area at an applied field of 10.31 V/μm.

This is a milestone achievement for Blue Phases in the first ever demonstration of them being used for wavefront modulation. Moreover, these devices were built on a PCB substrate with no intermediary layer, furthermore forming the first demonstration of Blue Phases grown on PCB. This significantly broadens the horizons of Blue Phase Liquid Crystals emerging as a multi-phase solution with high performance and approachable prototyping.

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Electrically Switchable vari-focal Continuous Phase Liquid Crystal Fresnel Zone Plate

Zhiyu Xu[1] , Camron Nourshargh, Tessar Wang, Nathan Spiller, Urban Mur, Alec Xu, Martin J. Booth, Steve J. Elston, and Stephen M. Morris.

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Lightweight, power-efficient, and electrically reconfigurable focusing optics are of growing importance for compact photonic systems, particularly in near-eye displays where optical efficiency and form factor are critical. Conventional liquid-crystal (LC) diffractive optics typically implement binary or multi-level phase steps, which inevitably distribute optical power into unwanted diffraction orders and can limit the achievable focusing efficiency. We present an electrically switchable *continuous-phase* Fresnel zone plate (FZP) realized by two-photon polymerization direct laser writing inside a polymerizable nematic LC cell (Figure 1), enabling smooth three-dimensional phase sculpting without reliance on photoalignment layers [1]. The design workflow converts a target wrapped lens phase profile into a spatially varying polymerization height distribution using an Euler–Lagrange-based director relaxation model, linking local director tilt and effective refractive index to optical phase retardation. This yields a continuous “kinoform-like” phase profile implemented as a polymer-stabilized director field embedded within an otherwise voltage-tunable LC layer. We demonstrate how dual-state focal switching can be achieved, which is further validated by imaging a resolution target in a 1:1 configuration (object and image planes at 2f*),* demonstrating practical voltage-addressable refocusing without the need for mechanical motion.

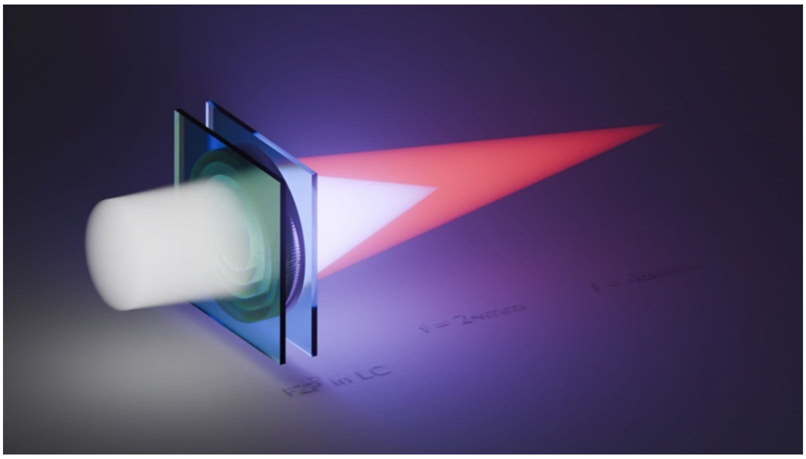

Figure 1. A switchable continuous-phase Fresnel Zone Plate.

[1] Z. Xu et al. Electrically switchable continuous phase liquid crystal Fresnel zone plate *Light: Science & Applications* (2026)

Adaptive Coherence Control for Holographic Measurement Systems using a Liquid Crystal Coherence Modulator

Tianxin Wang, Nathan P. Spiller, Steve J. Elston, Martin J. Booth, and Stephen M. Morris
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Lasers are ideal light sources for holographic measurements due to their high spatial and temporal coherence. In holography, good temporal coherence is required to maintain high-contrast and well-defined interference signals under finite optical path differences. However, when both spatial and temporal coherence are high, strong speckle noise inevitably appears after transmission through complex phase objects or reflection from surfaces with fine microstructures, degrading measurement quality.

A highly desirable solution is to preserve temporal coherence while selectively reducing spatial coherence. Towards this end, we report a novel liquid crystal coherence modulator (LCCM) that electrically induces fluctuations in the local refractive index leading to dynamic scattering states, which in turn result in rapidly varying speckle patterns without any mechanical motion. Compared with conventional approaches such as rotating diffusers and vibrating optical fibers, the proposed LCCM produces finer dynamic speckle on a sub-microsecond timescale, which effectively reduces spatial coherence, enabling sufficiently uniform illumination, while maintaining excellent temporal coherence. We demonstrate the integration of the LCCM into both transmission and reflection holographic measurement systems (Figure 1), enabling clear and accurate phase extraction for highly scattering biological samples and reconstruction of the surface morphology for non-planar surfaces. These results confirm that the proposed LCCM provides an effective, compact, and motion-free solution for speckle suppression in holographic measurement systems.

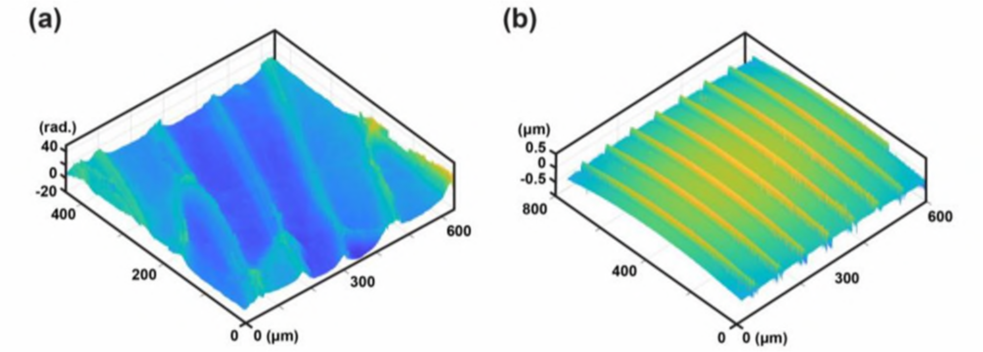

Figure 1. Reconstructed optical phase images of (a) onion cells and (b) etched grating structures.

Design Principles of Fluid Molecular Ferroelectrics

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Discovered in 2017, fluid molecular ferroelectrics are an emerging new class of organic materials where ferroelectricity is found in conjunction with true 3D fluidity whilst still retaining spontaneous polarization values comparable to their traditional solid-state counterparts [1,2]. Fluid molecular ferroelectrics are liquid crystalline (LC), with the majority of materials possessing nematic-like ordering of their constituents, thus this phase is termed the ferroelectric nematic, or N_F, phase (Fig. 1a) – but ferroelectricity has also been shown to exist in other traditional LC phases such as the smectic A and smectic C phases (SmA_F and SmC_p, respectively (Fig. 1b and c)). Fluid molecular ferroelectric materials are comprised of small organic molecules which currently exist in a constrained area of chemical space. This lack of structural diversity is largely due to a lack of understanding as to the molecular origins of ferroelectricity in these systems, making assigning true design rules for the preparation of fluid ferroelectrics difficult.

Here, we present a systematic study through the synthesis of some 100 highly fluorinated compounds based on three structure types [3-5]. By analogy with solid state molecular ferroelectrics, we shown H/F substitution to be a powerful and versatile tool for controlling ferroelectric order in fluid molecular systems [5]. In particular, specific fluorination patterns allow not only the thermal stability of the ferroelectric phase to be tuned, but also the nature of ferroelectric phase itself, determining whether nematic or smectic order is realised. We combine our physical findings with computational methodologies, such as atomistic MD simulations and DFT calculations, to help provide a set of ground rules to inform the design of future fluid molecular ferroelectric materials with specific properties, allowing for the production materials towards specific practical applications [6].

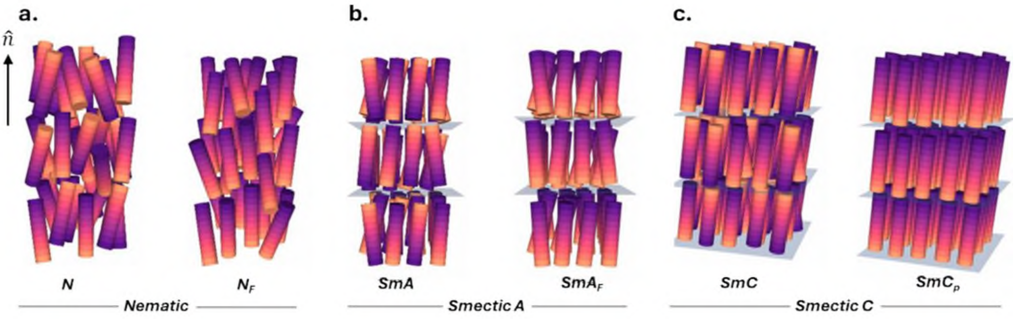

Fig. 1. Schematic representations of the para- and ferroelectric (a) nematic (N); (b) smectic C (SmC); and (C) smectic A (SmA) phases. Each rod is representative of a single molecule with the colour indicating the molecular direction.

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Modulated Anti-Ferroelectric Smectic Phases with Orthogonal and Tilted Structures

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The discovery of the ferroelectric nematic phase has brought with it a plethora of previously unobserved phases including nematics [1], smectics [1] and those that form spontaneously chiral structures [3,4]. In this contribution we will present evidence for the discovery of yet more novel phases, where modulated structures perpendicular to the layer normal form.

Evidence for these modulations is presented via X-ray scattering and shows that these modulations are stable in both orthogonal and tilted smectic phases before often transitioning to a helical phase. Various possible structures for antiferroelectric smectic A and C phase will be discussed as well as evidence that the modulated structures can be found in phases where the polarisation is not fully compensated as for anti-ferroelectrics.

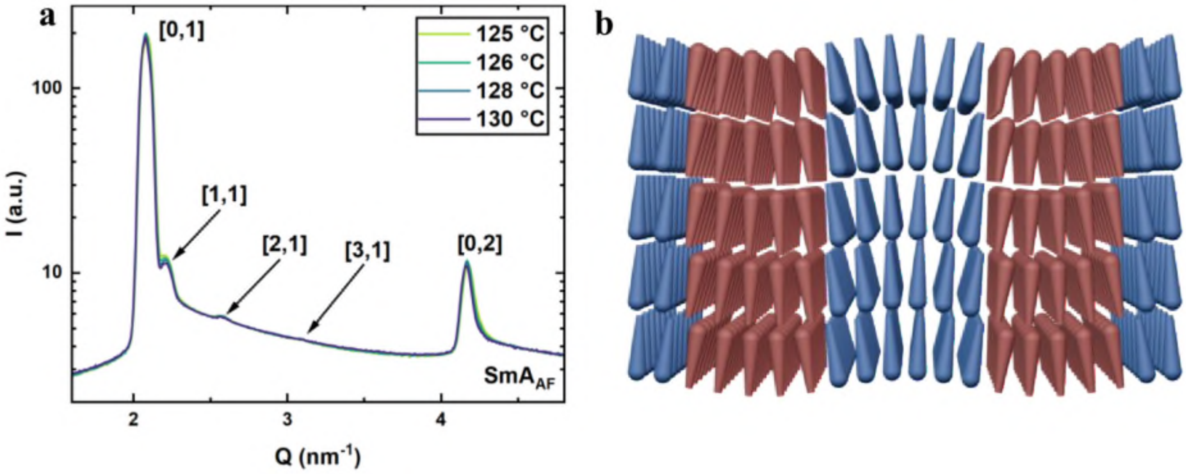

Figure 1. a) X-ray scattering data for the SmA$_{AF}$ phase showing satellite peaks due to modulation. b) proposed structure of the SmA$_{AF}$ phase.

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Computational approach for rapid screening for ferroelectric order in nematogens

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Ferroelectric nematics are a fascinating phase of matter, in which molecules exhibit bulk alignment of dipoles. There are, however, only a limited number of materials that have been discovered that show this phase. Moreover, small changes in structure can make or destroy ferroelectric behaviour.

Atomistic molecular dynamics simulations can be used to simulate ferroelectric liquid crystal phases [1]. Such calculations are sensitive to small changes in molecular structure and can provide a detailed representation of molecular order in addition to phase behaviour [1-4]. However, calculations of bulk liquid crystals are computationally expensive requiring many CPU days on parallel computers.

It is interesting to ask whether the interactions responsible for ferroelectric behaviour are captured in the interactions between pairs of molecules, or whether ferroelectric behaviour is an emergent property that arises from the interaction of molecular ensembles.

Here, we report a simple computational chemistry assay to screen for ferroelectric behaviour. Either a 3d chemical structure or a SMILES representation of a molecule is provided as input, and the automated script produces a molecular force field, generates a set of trial inputs for N mesogens in a non-polar environment, carries out 300 separate molecular dynamics runs and analyses the configurations to determine a preference (or otherwise) for ferroelectric ordering. The screen is rapid, taking just a couple of hours for each molecule. We test systems of 2, 6, 12 and 24 molecules.

In all cases, a clear preference for parallel or antiparallel dipole correlation can be detected through the simulation of just a small number of molecules, through the sign of the first peak of the distance-dependent dipole correlation factor, $g1(r)$. For most molecules, this is also seen for just two molecules (i.e. $N = 2$). While this simple computational screen cannot predict whether a nematic phase is stable or provide phase transition temperature predictions, it is nonetheless effective in providing good predictions for whether a molecule can form a polar nematic phase.

It is interesting to further ask whether this screen can be extended to provide simple computational measures to understand the tendency of molecules to form nematic and smectic phases. These measures can be used in machine learning approaches to predict bulk phase behaviour. Such studies are underway in our laboratory.

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Dipoles, boundary conditions, and the ferroelectric nematic phase

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In 1916, Born [1] proposed that dipole-dipole coupling provided the driving force for ferroelectric nematic (NF) formation. In the following years, however, theoreticians advanced precisely the opposite view, arguing that dipole-dipole interactions destabilised the NF phase [2]. Recently, Osipov [3] showed that boundary effects could affect the properties of an NF phase and possibly its very existence. Furthermore, recent experimental results [4] have shown that ferroelectric nematic liquid crystals, under certain conditions, spontaneously form helical structures, as predicted by Khachaturyan [2].

Atomistic simulations generally use the Particle Mesh Ewald sum technique to treat dipole-dipole interactions, but boundary conditions come into play here also [5]. Conducting, or "tin foil", boundary conditions are standardly used, but to our knowledge the effects of using other boundary conditions, such as an insulating boundary, have not been studied.

To study the effect of boundary conditions on the stability of the NF phase, we present simulation results for a classical Heisenberg spin lattice model [6] with additional dipole-dipole interactions [7], [8] . We will show that the resulting structure depends on the relative permittivity, , at infinity, with tin-foil boundary conditions ( ) resulting in polar ordering, while insulating boundary conditions ( ) result in a twisted helical structure. Additionally, at intermediate values, there is a phase transition between the polar and twisted structures, where the location of this transition is strongly dependent of the size of the simulation box.

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Frustrated Smectic Liquid Crystal Elastomers as Multifunctional Mechanical Metamaterials

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Liquid crystal elastomers (LCEs) are lightly cross-linked polymer networks, that display liquid crystalline character due to the incorporation of anisotropic units known as mesogens into their structure. Auxetics are materials that show a negative Poisson's ratio, i.e. thickening when under strain, which have found application in everyday items, such as sports equipment [1]. The discovery of nematic liquid crystal elastomers (LCEs) as molecular auxetic materials [2] was a paradigm-shift in the design of mechanical metamaterials as they are tuneable [3], transparent [4], scalable [5], non-porous and facile to fabricate.

All of the nematic auxetic LCEs reported thus far are side-chain LCEs, in which the mesogens are attached to the polymer backbone via a flexible spacer [2-6], and the nematic order is generally imparted on the LCEs by polymerisation in the nematic phase of the precursor mixture. Recently, we have shown that for precursors with significant structural similarity to those used to fabricate nematic auxetic LCEs, despite polymerisation being conducted in the nematic phase, smectic A LCEs are obtained [3,7]. Further analysis of the resulting smectic LCEs evidenced that the LCEs adopt a frustrated structure, with correlation lengths spanning short distances (<5 layers) [7]. This frustration results in LCEs showing a unique combination of properties, with some aspects of their behaviour characteristic of nematic LCEs, and others of smectic LCEs.

Here, we report for the first time that these frustrated smectic LCEs can display auxetic behaviour, expanding known synthetic molecular auxetics to a second family of LCEs [8]. Using theory proposed by Adams and Warner [9], we rationalize why only some of these frustrated LCEs are able to show an auxetic response, and others consistently fail prior to reaching the auxetic regime. In addition to the auxetic response, we examine the shear moduli of the frustrated smectic LCEs, which are an indicator as to their adhesive properties. The application of nematic LCEs as pressure-sensitive adhesives is an area of growing interest [10], thus here we report the first investigations into the adhesive prospects of these frustrated smectic LCEs.

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Mechanically reconfigurable auxetic metamaterials based on shape memory effect

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Auxeticity is a counterintuitive yet fascinating mechanical response where a material exhibits a negative Poisson's ratio, i.e. expansion rather than contraction is observed under uniaxial strain. Re-entrant auxetic metamaterials have been known for decades[1], but the first molecular-level auxetic system was realized in 2018 in a liquid crystal elastomer (LCE) by Mistry et al.[2]. The system has been demonstrated in transparent films of thickness ~100 μm, with the thickness limited by the need for high-quality monodomain alignment. As a rising-star material, significant scope remains for realizing both tunability and reconfigurability in auxetic LCEs. This work presents a mechanically reconfigurable auxetic LCE that uses the shape memory effect that can be imparted by introducing dynamic bonds into the LCE[3]. After partially replacing the covalent crosslinkers with physical hydrogen bonds, both the material shape and molecular alignment can be reprogrammed. An initially isotropic LCE sample is aligned through ~60% strain at ~100°C to form a monodomain smectic phase, with an order parameter ~0.59± 0.03. The alignment is stable after cooling to room temperature. Remarkably, this smectic LCE can be strained to over 1.0 and it exhibits an auxetic response[4] above a threshold strain of ~1.05 ± 0.05. The temporary network can be refreshed by heating to temperatures above 130°C and the reconfiguration process can be repeated several times. We show multiple alignment states that can be achieved via this reconfigurable mechanism and characterize the auxetic responses. This work demonstrates the first reconfigurable auxetic LCE, eliminating the conventional limitation of auxetic films to thicknesses of ~100 μm.

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Diverse helical structures made of achiral mesogenic dimers

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The formation of chiral structures from achiral building blocks and the propagation of chirality across length-scales in soft matter are still poorly understood phenomena. Since the first experimental observation of the twist-bend nematic (N_{TB}) phase in 2007 [1,2], much work has gone into studying the structure property relationships that govern the formation and stability of the phase. During these investigations, a variety of new helical smectic phases have been discovered, including the single helix ($SmC_{TB\text{-}SH}$) and double helix ($SmC_{TB\text{-}DH}$) phases [3,4] – as well as a newly reported intercalated helical phase ($SmC_{TB\text{-}C}$) [5]. These new phases piqued interest due to their longer and potentially tuneable helical pitch length when compared to the N_{TB} phase [6]. Investigation into this has included the synthesis of several new series of dimers with structural changes to the nature and size of mesogenic groups, the central spacer, and the terminal chain length.

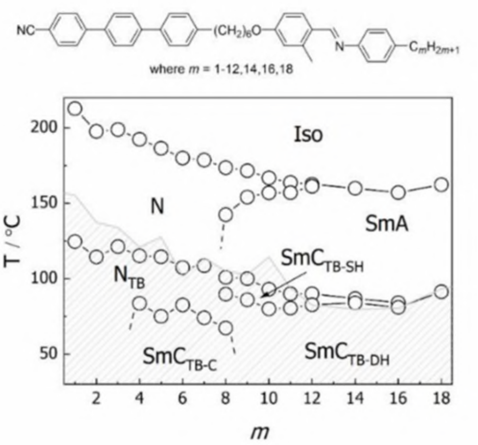

Figure 1: Molecular structure and a phase diagram for the CT6O2Me.m series. Grey hashed area marks the region of monotropic phase behaviour.

Here we present new series of liquid crystal dimers consisting of cyanoterphenyl and benzylideneaniline based mesogenic units linked by a flexible alkyl spacer which exhibit both the $SmC_{TB\text{-}SH}$ and $SmC_{TB\text{-}DH}$ phases, as well as other helical intercalated and bilayer phases. Through characterisation of these series using techniques such as X-ray diffraction, polarised optical microscopy and measurements of the optical birefringence, it was observed that heliconical ordering was preserved in the newly reported $SmC_{TB\text{-}C}$ phase, despite the molecular intercalation strongly supressing azimuthal rotation of the director.

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Synthesis and characterisation of liquid crystals bearing a sustainable novel uracil derived headgroup

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Liquid crystals (LC's) are a state of matter combining the orientational order of the solid state with the fluidity of the liquid phase and are best known for being catalysing the digital revolution as our principle means of information display through their use in liquid crystal display technology (LCD's). Liquid crystals employed in such use cases are rod-like materials (calamitic) which exhibit different liquid crystalline (or mesophases) based on temperature (i.e. thermotropic). These are typically all derived from petrol chemicals, with less than 3% liquid crystal having any reference to sustainable chemistry or its practises.[1]

Arguably, the most commonly used mesogenic materials used contain a cyanobiphenyl (CB) moiety due to its highly polar and polarizable nature helping to drive mesophase formation. A replacement for the CB function would therefore have to have similar pilar and polarizable properties. Uracil is a natural product containing a functionalised pyrimidine ring which meets both of the necessary criteria to be a viable replacement for the CB moiety. Uracil has green credentials as it has successfully been extracted from natural sources for over two centuries,[2,3] with synthetic routes from urea, 2,4-dimethoxypyrimidine, and deamination of cytosine shown to be also being possible.[3–5]

Herein, a number of LC materials bearing a novel uracil motif have been synthesised and their LC properties characterised. We find a mesonic core based on the uracil moiety to have similar properties to the CB unit. These materials exhibit such LC sub phases as the conventional nematic (N) phase (used in display technology) and the chiral nematic (N*) phase (used in sensing applications).

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Structure-Property Relationships of Polar Mesogens Containing Sulfur

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The ferroelectric nematic phase, NF, has become one of the most prominent topics in the field of liquid crystal research since its experimental discovery in 2017[1,2] and assignment in 2020.[3] The NF phase is a variant of the conventional nematic phase, N, which is the least ordered liquid crystalline phase and has been widely used in display devices. The NF phase has huge potential towards driving the next generation of devices because it requires a lower energy cost compared to existing technology due to the dipoles already being aligned.[4] To date there have been around a 200 low molar mass compounds which exhibit the phase[5] and the vast majority of these can be described using the three following structures, namely RM734,[1] DIO[2] and UUQU-4N[6], Figure 1. The observation of further new polar phases [7,8] has highlighted the need to continue the synthesis and characterization of new mesogens in this structure space. Here we report the transitional properties of a number of sulfur-containing compounds which exhibit both polar and non-polar phases and then investigate their structure-property relationships with regards to the stability of the observed polar phases.

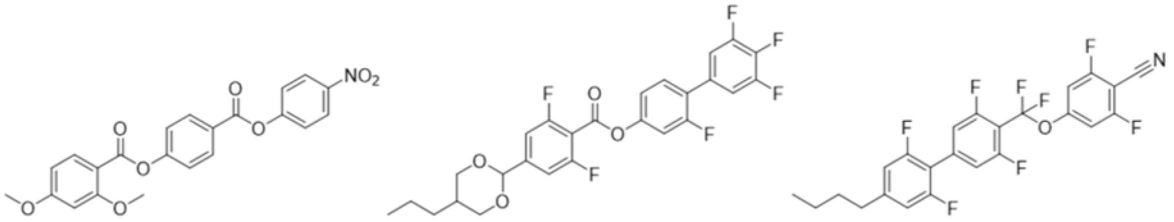

Figure 1. Molecular structure of (left) RM734, (middle) DIO and (right) UUQU-4N.

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Chevron Instability in Active Smectics as a Model for Muscle Tissue in Zebrafish

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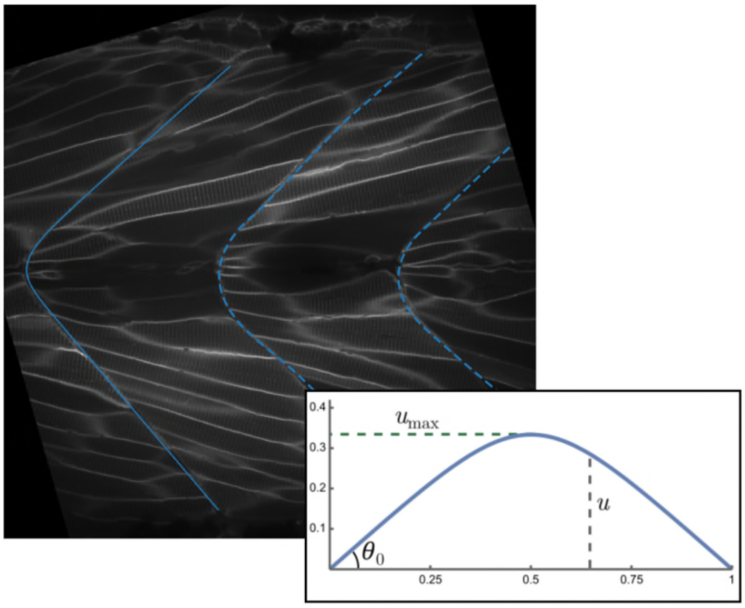
We study an active smectic liquid crystal system confined to a bookshelf geometry. It is found that above a threshold activity, the smectic layers are susceptible to a chevron-like instability which bears a striking resemblance to the characteristic chevron shape of the muscle segments found in the skeletal muscle tissue of zebrafish. Comparison of this theoretical model with experimental data taken from experiments on zebrafish allows for the determination of physical properties of the muscle tissue such as bending and dilation elastic moduli that would otherwise be inaccessible experimentally, and comparison of these moduli can in turn can be used to explain the morphological properties of the tissue at different stages of development.



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Towards the mesoscopic simulations of Liquid Crystal Elastomers

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Liquid Crystal Elastomers (LCE) are crosslinked polymer networks with anisotropy of LCs and elasticity. Our simulations have been developed using the new modelling tool - Morpho [1]. Morpho is able to handle both the shape and field changes along with the capacity to add boundary conditions which are crucial while handling LC materials. Applying Morpho simulations to LC tactoids [2] has verified its use in modelling LCs. Applying Morpho simulations to a rectangular elastomer sheet with a hole [3] has verified its use in modelling elasticity. We next move towards the modelling of LCEs by combining the free energies involved in modelling tactoids and elasticity. The LCE simulations involve minimisations of combined free energy [4,5] and data analysis of stress, strain, director and energy distribution. The study was done from a reference configuration with a preferred director profile to the resulting deformed state. The stress, strain, director and energy analysis were plotted and analysed. The developed model has promise to test new LCE geometries and to investigate parameter dependences as further research.

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Stability of Nematic Equilibria in Isosceles Triangular Domains

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Geometric confinement plays a key role in determining the equilibrium configurations of nematic liquid crystals. In particular, triangular domains provide a natural setting to investigate how domain geometry influences defect structures and stability. In this work, we study nematic equilibria in isosceles triangular domains using the reduced Landau–de Gennes model. The model describes the orientational order through two components of the reduced Q-tensor, q1 and q2, satisfying a coupled system of partial differential equations with Dirichlet boundary conditions enforcing tangent alignment along the triangle edges.

Our study investigates the influence of the rescaled edge length λ and the apex angle of the isosceles triangle, on the resulting nematic configurations. Finite element simulations are performed using COMSOL Multiphysics to compute equilibrium solutions and analyse their behaviour.

The results show that the geometry of the domain strongly affects the location of defects, which correspond to regions of reduced nematic order. For small apex angles, defects tend to appear near the base of the triangle, while for wider apex angles the defects move towards the apex. In addition, increasing the elastic parameter λ increases the degree of nematic order throughout the domain. These results provide insight into how geometric confinement can be used to control defect locations and nematic ordering in confined liquid crystal systems.

Nematic Liquid Crystal Configurations in Triangular Confinement

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Nematic liquid crystals confined within polygonal domains provide a rich framework for exploring how geometry influences structural phase transitions and defect formation. Among these shapes, triangles offer the simplest setting in which confinement and geometric frustration can be studied. Isosceles triangles are of particular interest because they can be parametrised by an edge length, λ, and an apex angle, θ, and can be readily fabricated in experimental settings.

In this work, we study nematic equilibria in isosceles triangles using a two-dimensional reduced Landau-de Gennes framework with tangential boundary conditions. Using a Schwarz-Christoffel mapping approach, we compute the unique nematic equilibrium in the $\lambda \to 0$ limit (for small systems). We obtain an explicit relationship between the apex angle and the number and locations of interior defects.

In the opposite regime of large systems ($\lambda \to \infty$), we investigate multistability as a function of the apex angle. We also extend our study to saddle points of the reduced Landau-de Gennes free energy to understand the connectivity between different stable configurations in this limit.

Together, our results highlight how tuning the apex angle provides a simple mechanism for controlling defect positions and modulating the number and type of stable nematic configurations in triangular confinement. This is joint work with Prof Apala Majumdar and Prof Andrew Hazel.

Control of a Dual-Frequency Liquid Crystal Variable Attenuator for the Power Stabilisation of a Terahertz Quantum-Cascade Laser

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The terahertz (THz) band is a section of the electromagnetic (EM) spectrum that sits between microwaves and the infrared. It is 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].

Liquid crystals (LCs) have shown promise in the THz band for the use in adaptive optics (AOs) [2], an area of THz research that is still emerging. However, due to the much longer operating wavelengths than infrared/visible bands, THz LC devices are required to be much thicker, which greatly increases switching times. To overcome this, we use a dual-frequency LC (DFLC), a type of nematic LC whose dielectric anisotropy,

$\Delta\varepsilon$, changes with the frequency of the applied bias. Typically, for a driving frequency of 1 kHz $\Delta\varepsilon$ is positive, and negative for higher frequencies (>20 kHz). This property allows for two driven perpendicular states, greatly speeding up the operation of thick devices.

We have fabricated a variable attenuator using a DFLC optimised for a 3.2 THz quantum-cascade laser (QCL) system. While varying the bias frequency can control the orientations of the DFLC molecules, it is not a useful control for a variable attenuator. At the crossover frequency $\Delta\varepsilon \rightarrow 0$ and switching time between states becomes large. We implement a dual-tone control signal that applies two frequencies simultaneously and varies the ratio of their amplitudes. As can be seen in Fig. 1(a), a switching effect occurs over a narrow range of ratios and is ideal for the use in a power stabilisation system. This device has been integrated into a hardware-based power stabilisation system and tested with a 3.2 THz QCL. Fig. 1(b) shows the DFLC device varying the THz power in order to track a sine wave which operates with a greater speed and amplitude than the expected variations created by thermal power drifts of a QCL (on the order of a few percent [3]).

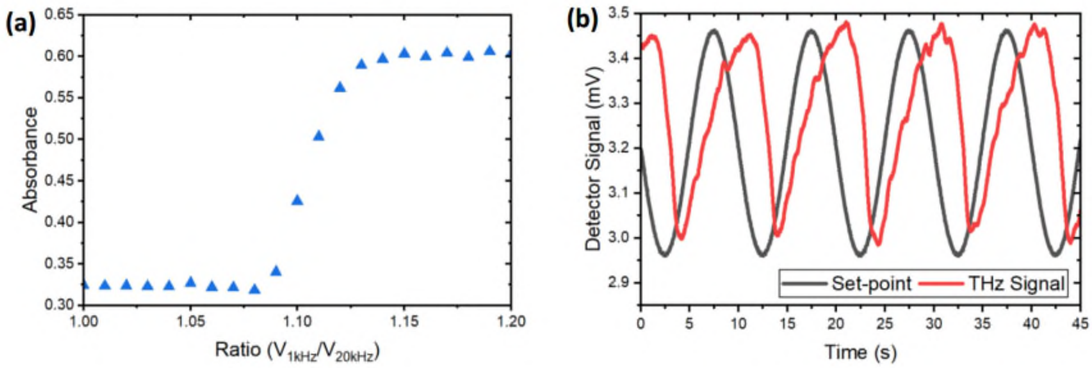

Fig 1. (a) Processed THz-Time Domain Spectroscopy data showing the change in THz absorbance of the DFLC device as a function of bias ratio. (b) The DFLC device in a PI loop controlling the power of a THz QCL to follow a sine wave

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FROM BPIII TO HELIX INVERSION: MESOMORPHIC BEHAVIOUR AND CHIRALITY TRANSFER IN CHIRAL MESOGENIC DIMERS

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Chirality plays a fundamental role in the self-organization of liquid crystalline materials, giving rise to a variety of complex supramolecular structures such as cholesteric and blue phases.1 In chiral systems, molecular asymmetry can induce long-range helical organization, while subtle variations in molecular structure may significantly influence mesophase stability and chirality transfer. Mesogenic dimers are particularly attractive model systems in this context because their conformational flexibility often leads to rich mesophase behaviour and unusual chiral phenomena.2

In this work, a homologous series of chiral mesogenic dimers containing a phenyl-3-hydroxypropanoate unit as a source of chirality and terminal alkyl chains of different lengths was investigated (Figure 1). The compounds were synthesized in both racemic and enantiomerically pure forms in order to examine the influence of chirality on mesomorphic behaviour.

The effect of terminal chain length on mesophase formation, including the appearance of BPIII, will be presented. Particular attention is given to chirality transfer to various achiral nematic hosts and the induction of helix inversion in these systems. The results provide insight into the interplay between molecular structure, chirality, and supramolecular organization in chiral liquid crystal systems.

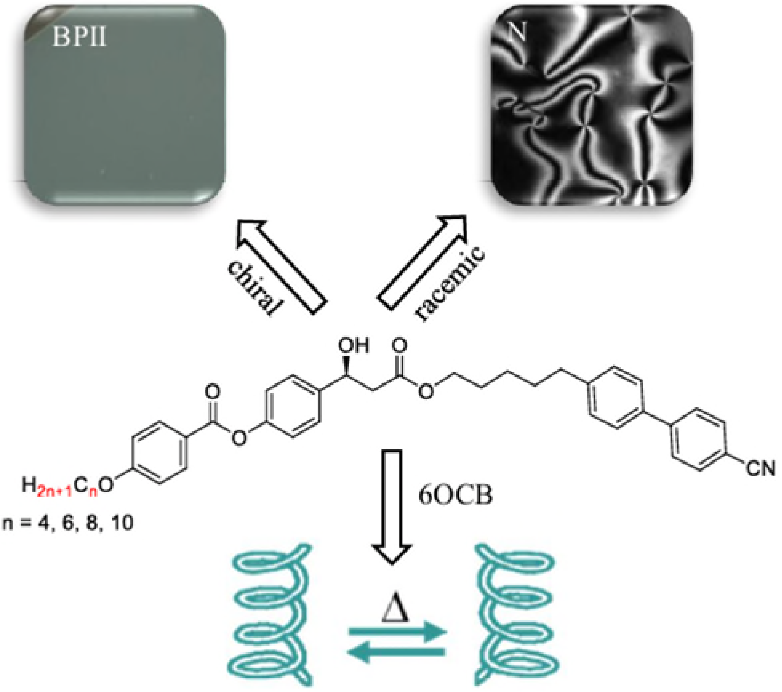

Figure 1. Molecular structure and the characteristic mesomorphic behaviour of the synthesized dimers

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Multidimensional, Multilevel Information Storage and Encryption in Auxetic Liquid Crystal Elastomers

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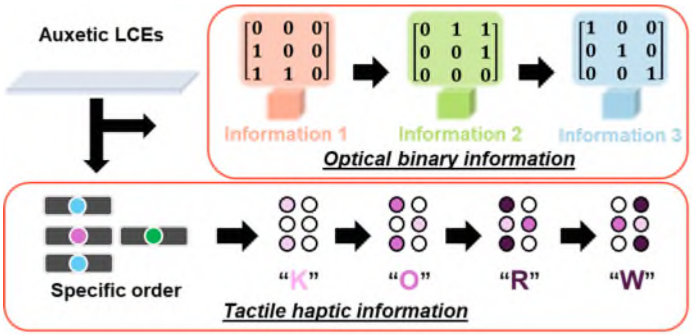
Auxetic metamaterials exhibit negative Poisson's ratio, where the materials expand rather than contract under uniaxial strain. Re-entrant auxetic metamaterials have been widely utilized in versatile scenarios, like indentation resistance and energy absorption for decades1, while the very first molecular level auxetic material, a liquid crystal elastomer (LCE), was synthesized by Mistry *et al.* in 2018.2The optical and morphology features that occur in a LCE during the auxetic response3offer interesting potential for information applications. In this work, we present a novel and facile strategy to achieve multidimensional, multilevel information storage and encryption (M2ISE) with auxetic LCEs.4E-field alignment of the precursor mixture is used to manipulate the director in the plane of the elastomer film. A small voltage (≤ 2.00 Vrms) can tune the threshold strain of the auxetic response within the range of ~0.58 ± 0.05 to ~0.91 ± 0.05. Based on the distinct optical and morphological properties of these tuned auxetic responses, we have realized M2ISE for not only 2D optical information but also 3D tactile information. This study paves a new way for the development of encryption in soft materials with high security and versatility for extensive applications.



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Synthesis and Characterisation of Fluorinated Ferroelectric Nematogens

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The ferroelectric nematic phase, NF, has been of significant research interest since its identification in 2020. The initial discovery of this phase can be attributed to two independently but simultaneously published materials: RM734 [1] and DIO [2]. The NF phase has demonstrated a host of highly desirable electro-optical properties, including extraordinarily high polarisation values, and dielectric anisotropies several hundred times larger than those of conventional nematogens [1-3]. RM734 and DIO, as well as the subsequently discovered UUQU-4N [4] (Figure 1) form the archetypal structures that the vast majority of ferroelectric nematic liquid crystals are based on to date. However, while upwards of 300 molecules have been investigated to date, it is not yet well understood what combination of structural features best support the appearance and stability of the NF phase. We aim to deepen the understanding of these structure-property relationships through the synthesis and characterisation of new ferroelectric nematogens.

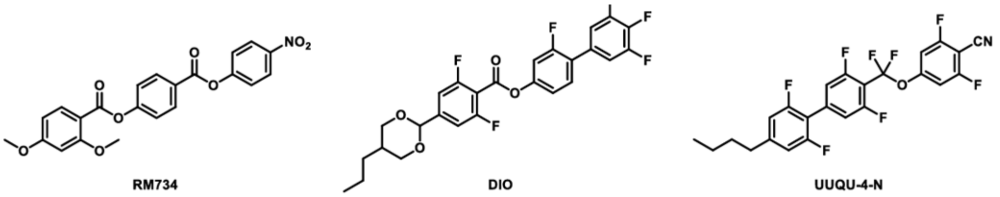

Figure 1. Structures of the archetypal ferroelectric nematogens: RM734, DIO and UUQU-4-N.

In the present work, we combine some of the characteristic chemical motifs of RM734-type and UUQU-type structures to create new ferroelectric nematogens with a highly fluorinated mesogenic core. By varying structural features within these series, such as the degree of molecular biaxiality - by variation of the position and length of lateral alkyl chains - the effect of these alterations on the stability of this fascinating phase of soft matter will be assessed.

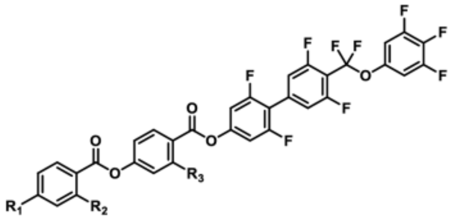

Figure 2. General structure of series presented in this work, where R = H or O-CnH2n+1, with the value of n ranging from 1-5

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Acoustic control of soft matter-based composites

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Polymer composites combine the lightweight and corrosion resistant properties of polymers with the enhanced strength and functional properties of dopant materials such as magnetite nanoparticles. This combination enables the creation of advanced materials with tailored mechanical, thermal, and electromagnetic properties for applications in high-value sectors such as aerospace, construction, and renewable energy. Precise control over properties such as directional thermal conductivity, would transform applications such as thermal management solutions. Realising such control requires accurate control of dopant distribution and orientation, particularly for anisotropic particles, which can be achieved using acoustic alignment[1-3].

Initial modelling and experimental work has been performed to explore the shape of the ultrasound field produced for different container geometries and determine the ultrasonic power required for particle alignment. An ultrasound horn at 40kHz is used to generate surface acoustic waves in a substrate which leads to acoustic tweezing. Figure 1(a) and (c) show the experimental alignment of solid particles in water and air bubbles in Norland optical adhesive respectively. Figure 1(b) shows alignment of the solid particles in water for a square geometry with the ultrasound generation positioned in the corner.

Modelling predicts that an increase in fluid layer thickness results in reduced acoustic power and therefore alignment of particles. This has been confirmed experimentally. Other contributors are particle size, density, fluid viscosity and frequency (velocity gradients).

Figure 1. Ultrasonic alignment of solid particles in water for (a) a circular geometry and (b) a square geometry, and (c) alignment of bubble in Norland optical adhesive.

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