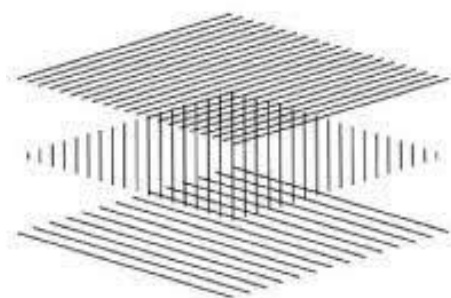


British Liquid Crystal Society

Annual Meeting 2024
10th – 12th April - Oxford

Book of Abstracts

Hosted by the University of Oxford



BRITISH
LIQUID
CRYSTAL
SOCIETY



Photo Credit: Dr Ben Outram

Active nematics: A new approach to mechanobiology?

Julia M. Yeomans

The Rudolf Peierls Centre for Theoretical Physics, Clarendon Laboratory, University of Oxford, Parks Road, Oxford, OX1 3PU, UK

Active materials such as bacteria, molecular motors and eukaryotic cells continuously transform chemical energy taken from their surroundings to mechanical work. Dense active nematics show mesoscale turbulence, the emergence of chaotic flow structures characterised by high vorticity and self-propelled topological defects. I shall describe the physics of active nematics and discuss how this may be relevant to biological processes such as cell sorting and early embryogenesis.

The Role of Activity Patterning in Active Nematic Flow Transitions

A.J.H. Houston* and N.J. Mottram

School of Mathematics and Statistics, University of Glasgow, University Place, Glasgow, G12 8QQ

*alexander.houston@glasgow.ac.uk

Active nematics model a wide range of living systems, including cells layers and bacteria [1]. However, real biological systems will not have uniform activity, either due to population variance or due to the presence of distinct species or cell types. As well as arising naturally, it has been recently demonstrated that the structure of activity in a material can be controlled through modulating light intensity [2]. This provides motivation to understand the effects of activity patterning, both to gain insight into the in vivo behaviour of biological systems and to open up routes to engineer desired dynamics in active matter. One of the hallmarks of active nematics is that, when confined to a channel, they will transition to a flowing state once above a threshold activity [3], and it is in this context that we study the role of activity patterning. The system is described by an operator that is non-Hermitian and non-local, both features that complicate the analysis. We provide a solution for an arbitrary piecewise-constant activity profile. From this we show that patterning allows a significant reduction in the net activity required for a flow transition and also makes it possible to control the structure of the flowing state. A simple instance of this is illustrated in Figure 1.

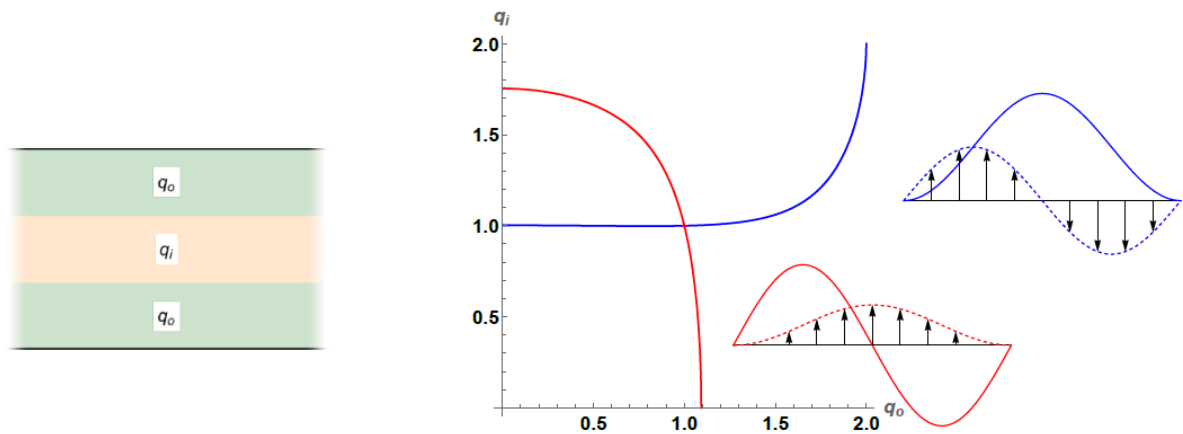


Figure 1: Left: a symmetric three-layer activity pattern. Right: the corresponding phase space for flow instabilities. The insets show the director (solid) and flow (dashed with arrows). When the activity is higher at the edges the red mode becomes unstable, while the blue mode results when the activity is higher in the middle.

References

- [1] A. Doostmohammadi Nat. Commun. **9**, 3246 (2018)
- [2] R. Zhang, et al., Nat. Mater., **20**, 875–882 (2021)
- [3] R. Voituriez et al., EPL **70** 404 (2005)

On the thermodynamics of biaxial nematics with discrete orientational degrees of freedom

Giovanni De Matteis^{1,2}, **Francesco Giglio**^{3*}, and Antonio Moro³

¹ Dipartimento di Matematica e Fisica, Università del Salento, Lecce, ITA.

² I.N.F.N. Sezione di Lecce, Lecce, ITA.

³ School of Mathematics and Statistics, University of Glasgow, Glasgow, UK.

⁴ Department of Mathematics, Physics and Electrical Engineering, Northumbria University Newcastle, Newcastle upon Tyne, UK.

UK.*Francesco.Giglio@Glasgow.ac.uk

Phase transitions in macroscopic systems at the equilibrium have shown to be intimately related to the theory of nonlinear conservation laws. Examples range from simple systems like van der Waals fluids, uniaxial and biaxial Nematic Liquid Crystal models and spin systems to complex systems such as Random Matrix models. In such models, order parameters fulfil suitable nonlinear PDEs with prescribed initial conditions and phase transitions are explained in terms of shock waves travelling in the space of control parameters (e.g. thermodynamic variables).

The talk aims at presenting recent results [1], obtained within the above framework, in the context of biaxial nematics. In particular, we study a discrete version of the Maier–Saupe model for nematic liquid crystals and propose a biaxial generalization, i.e. Straley model, further extended to account for the effects of external fields. In the thermodynamic limit, we derive an explicit set of four equations of state for the orientational order parameters, which are identified with Gibbs weights of the statistical model. Focusing our study on the thermodynamics in the absence of external fields, we show that the system is fully characterised by two scalar order parameters. The resulting zero-field phase diagram is discussed in terms of the intrinsic biaxiality of the interaction and the temperature, and the corresponding order parameters behaviour is analysed. Two-parameter reductions accounting for the presence of external fields are also derived, hence providing an outlook towards possible future works and applications. Finally, we show how our findings are consistent with known results in the literature.

References

[1] De Matteis G, Giglio F, Moro A. 2024 Complete integrability and equilibrium thermodynamics of biaxial nematic systems with discrete orientational degrees of freedom. Proc.R.Soc.A480: 20230701.<https://doi.org/10.1098/rspa.2023.0701>

Evidence of order-disorder ferroelectric behaviour in NF materials

Thomas Raistrick¹, Richard J. Mandle^{1,2}, Zhaopeng Zhang¹, Peter J Tipping¹, and Helen F Gleeson¹

¹ *School of Physics and Astronomy, University of Leeds*

² *School of Chemistry, University of Leeds*

In 2017, the ferroelectric nematic phase (NF) was observed, more than a century after it was first theoretically predicted. [1-3] The ferroelectric nematic phase exhibits polar ordering $\hat{n} \neq n$ where n is the nematic director, in contrast to the ordinary nematic phase (N), which is apolar. The fundamental interest in the NF phase as a polar, ordered fluid system is enhanced by the reports of these materials exceptionally large dielectric permittivities and spontaneous polarization values. [3] As such ferroelectric nematics are expected to have far-reaching applications in non-linear optic devices, fluid capacitors for energy storage and photonic devices. [3-4] For these reasons, in addition to the fundamental interest in understanding the behaviour of a polar nematic fluid, it is of utmost importance to understand the order parameters within the phase.

In this talk, we report the uniaxial order parameters of RM734, one of the first examples of the ferroelectric nematic phase, as determined via Raman spectroscopy and birefringence measurements. The findings are interpreted by drawing parallels between the ferroelectric nematic fluid phase and solid-state ferroelectric materials. It is suggested that the existence of polar order, and/or a change in the reorientational dynamics of the molecules, at the onset of the NF phase may be reflected in the changes in the full-width half maxima of the Raman signal. The energetic barrier of the transition from the para-electric to ferro-electric phase is found to be of the order of 2.5 ± 0.6 kJ/mol, which is considerably lower than the energetic barrier in solid ferroelectric materials.

References

- [1] M. Born, *Ueber anisotrope flüssigkeiten: Versuch einer theorie der flüssigen kristalle und des elektrischen kerr-effekts in flüssigkeiten*. 1916.
- [2] R. J. Mandle, S. J. Cowling, and J. W. Goodby, "A nematic to nematic transformation exhibited by a rod-like liquid crystal," *Physical Chemistry Chemical Physics*, vol. 19, no. 18, pp. 11429–11435, 2017.
- [3] H. Nishikawa et al., "A fluid liquid-crystal material with highly polar order," *Advanced materials*, vol. 29, no. 43, p. 1702354, 2017.
- [4] N. Sebastián et al., "Polarization patterning in ferroelectric nematic liquids via flexoelectric coupling," *Nature Communications*, vol. 14, no. 1, p. 3029, 2023.

Diving into Dimerland - Structure property relationship of liquid crystal dimers and the ferroelectric nematic phase

N. Tufaha^{1*}, D. Pocięcha², E. Gorecka², J.M.D. Storey¹, C.T. Imrie¹

¹ Department of Chemistry, University of Aberdeen, Aberdeen, U.K.

² Faculty of Chemistry, University of Warsaw, Warsaw, Poland

Ever since the experimental discovery of the ferroelectric nematic phase, NF, in 2017, a significant amount of research has been done to elucidate the structure-property relationships that govern the formation of this phase. This work has mainly involved the investigation of rodlike compounds [1] based on the general structures of the first ferroelectric nematogens reported RM734 [2], DIO [3] and UUQU-4-N [4].

In contrast to the conventional uniaxial nematic phase, N, in which the constituent molecules align along a common direction known as the director, n , which has inversion symmetry $n = -n$, in the NF phase, there is a spontaneous alignment of the molecular dipoles such that $n \neq -n$ and the phase is polar.

In 2023, however, it was reported that liquid crystal dimers could also show the NF phase. [5] The dimer investigated di-5(3FM-C4T), consists of mesogenic units having large dipole moments achieved using fluorine substitution and alternating regions of electron density. Furthermore, di-5(3FM-C4T) shows a ferroelectric SmAPF phase as seen for bent-shaped molecules. It is suggested that in order to allow for the formation of a polar phase, the bent molecules must adopt a U-shape and a polar head-tail character.

In this work, we investigate the structure-property relationship of liquid crystal dimers based on di-5(3FM-C4T), shown in Figure 1, in order to obtain a better understanding of the factors that direct the formation of the NF phase in more complex systems.

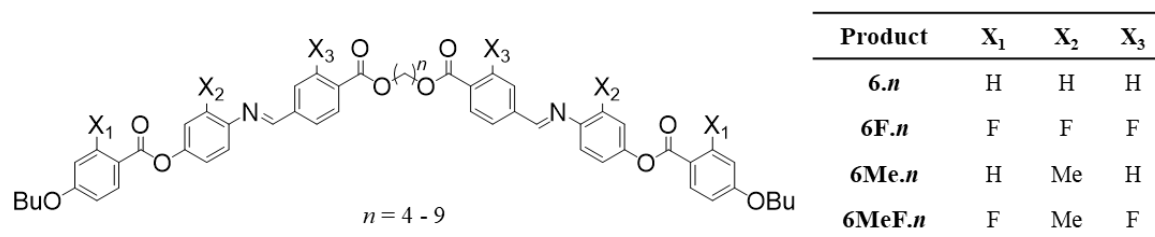


Figure 1. Structural modifications of di-5(3FM-C4T) presented in this work.

References

- [1] E. Cruickshank, Chempluschem 7:e202300726, (2024).
- [2] R. J. Mandl, S. J. Cowling, et al., Phys. Chem. Chem. Phys. 19(18), 11429–11435, (2017).
- [3] H. Nishikawa, K. Shiroshita, et al., Adv. Mat. 29(43), 1702354, (2017).
- [4] A. Manabe, M. Bremer, et al., Liq. Cryst. 48(8), 1079–1086, (2021).
- [5] S. Nakasugi, S. Kang, et al., J Phys Chem B 127(29), 6585–6595, (2023).

Deviations from Nematic Behaviour in Polar Nematic Liquid Crystals

K. Fagg¹, H. F. Gleeson¹, R. Mandle^{1,2}, M. Nagaraj^{1*}

¹ *School of Physics and Astronomy, University of Leeds, Leeds, LS2 9BW.*

² *School of Chemistry, University of Leeds, Leeds, LS2 9JT.*

**corresponding author email: m.nagaraj@leeds.ac.uk*

The experimental discovery of the ferroelectric nematic (Nf) liquid crystal phase in 2017 has since gained considerable attention for its use in fundamental and applied science [1,2]. The Nf phase has orientational order but does not possess an inversion symmetry, leading to a bulk polarity. To achieve this conformation, the molecules themselves also typically have a high polarity. How this molecular polarity manifests in the higher-temperature non-polar nematic phase (N) is an important consideration, and whether any N bulk properties are affected should be investigated.

We present the temperature-dependence of bulk properties in the nematic phase of a liquid crystal mixture (M5) that exhibits an enantiotropic Nf phase. These properties include the splay and bend elastic constants (K_{11} , K_{33}), dielectric permittivity, and the Freedericksz threshold voltage. On cooling, our results show an initial reduction in the values of K_{11} and V_{th} until approximately 8degC above the transition into the intermediary nematic (Nx) phase, after which these values drastically increase. Conversely, values for K_{33} and dielectric anisotropy increase with decreasing temperature and display similar trends to nematic materials 5CB and E7. At higher temperatures close to the nematic-isotropic transition, good fitting to nematic models is displayed, whereas lower temperatures approaching the transition into the Nx and Nf phases show strong deviations from these models.

A New Chemical Structure Space Exhibiting the Ferroelectric (NF) Nematic Phase

C. J. Gibb¹, J. L. Hobbs², and R. J. Mandle^{1,2}

¹ *School of Chemistry, University of Leeds, Leeds, UK, LS2 9JT*

² *School of Physics and Astronomy, University of Leeds, Leeds, UK, LS2 9JT*

* c.j.gibb@leeds.ac.uk

Since the practical discovery of the ferroelectric nematic (NF) phase at equilibrium in the late 2010's, the phase has garnered significant excitement prompting it to be studied extensively as it has been 'promised to remake nematic science and technology' [1]. Despite the work which has been carried out to date, studies into the NF phase are still in their infancy. The current materials being studied are all based on 3 archetypal structures: RM734 [2], DIO [3] and UUQU-4N [4]. These current materials present the unwelcome combination of challenging working temperature ranges and often low chemical stability. This has driven a significant appetite for new materials that can sustain the polar mesophase at and below ambient temperatures [5][6].

We report the synthesis and liquid crystal characterisation of some 60 new, highly fluorinated compounds based on a novel structure type. Of the 60 materials studied, some 30 of these materials are ferroelectric nematogens – the largest single study into the chemistry of the NF reported to date. Although some of these compounds melt and exhibit the NF phase close to ambient temperature (circa 40 °C), we achieve true room temperature example of the phase through the formulation of binary mixtures. Due to the novel structures reported, these mixtures are more chemically stable than previously reported mixtures, stabilising the NF phase over large temperature ranges.

References

- [1] O. D. Lavrentovich, PNAS 117, 14629 (2020).
- [2] R. J. Mandle, et al., PhysChemChemPhys, 19, 11429 (2017)
- [3] H. Nishikawa, et al., Advanced Materials, 29, 1702354 (2017)
- [4] A. Manabe, et al., Liq. Cryst. 48, 1079 (2021).

Stimuli-responsive Materials based on Liquid Crystal Polymers

Albert P. H. J. Schenning

Stimuli-responsive Functional Materials and Devices, Department of Chemical Engineering and Chemistry, Eindhoven University of Technology, P.O. Box 513, 5600 MB Eindhoven, The Netherlands

E-mail: a.p.h.j.schenning@tue.nl

Stimuli-responsive polymers which change their properties in response to a are one of the focal points in materials science. The self-assembly of liquid crystals has proven to be an extremely useful tool in the development of such smart soft materials. Liquid crystalline polymer materials are appealing as microscopic changes in the molecular order and orientation can lead to macroscopic changes in shape and optical properties. In my lecture, I will discuss stimuli responsive polymers based on liquid crystals that can be applied as soft actuators, robots, color changing materials and sensors (Figure 1).

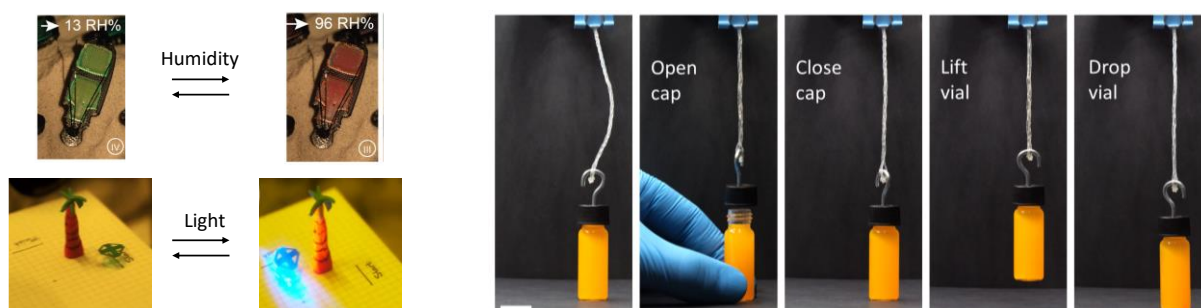


Figure 1. Examples of based on liquid crystal polymers which respond to temperature (right), humidity (top, left), and/or light (bottom, left) by changing their shape and/or color.

References

- [1] S.J.D. Lugger, S.J.A. Houben, Y. Foelen, M.G. Debije, A.P.H.J. Schenning, D.J. Mulder, *Chem. Rev.* **2022**, *122*, 4946-4975
- [2] M. Pilz da Cunha, M.G. Debije, A.P.H.J. Schenning, *Chem. Soc. Rev.* **2020**, *49*, 6568-6578
- [3] Y. Foelen, A.P.H.J. Schenning, *Adv. Sci.* **2022**, *9*, 2200399
- [4] P. Zhang, L.T. de Haan, M.G. Debije, A.P.H.J. Schenning, *Light Sci. Appl.* **2022**, *11*, 248

Structure-Property Relationships in Auxetic Liquid Crystal Elastomers

Stuart R. Berrow^{1*}, Thomas Raistrick¹, Richard J. Mandle^{1,2}, Helen F. Gleeson¹

¹ School of Physics and Astronomy, University of Leeds, Leeds, LS2 9JT.

² School of Chemistry, University of Leeds, LS2 9JT, UK

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

Auxetics are materials possessing a negative Poisson's ratio, i.e. they get thicker when subject to strain.[1] They typically consist of porous structures, with deformation of the pores during strain causing the auxetic response.[2,3] However, liquid crystal elastomers (LCEs) displaying auxetic behaviour have been reported, realizing the first examples of a non-porous, synthetic, molecular auxetic material.[4,5] The mechanism of the auxetic response is attributed to an out-of-plane rotation of the nematic director under strain, and a resulting emergence of biaxial character within the elastomer.[4,5]

The auxetic LCE can be described as predominantly a side-chain LCE, in which the mesogens are attached to the polymer backbone by a flexible chain known as a spacer. This gives three distinct molecular components that can be varied in order to tailor material properties: the backbone, the spacer, and the mesogen.[6-8] As yet, there have been no systematic studies of potential structure-property relationships in auxetic LCEs.

This work will discuss the synthesis of a series of acrylate monomers with, differing by variations in spacer length and mesogenic group, and their subsequent incorporation into liquid crystal elastomers of formulations consistent with the auxetic LCE previously reported. The impact of these changes on LCE properties such as the phase transition temperatures will be reported. Crucially, the impact of spacer length on the auxetic behavior of the LCEs will be addressed to further our understanding of the auxetic response in LCEs.

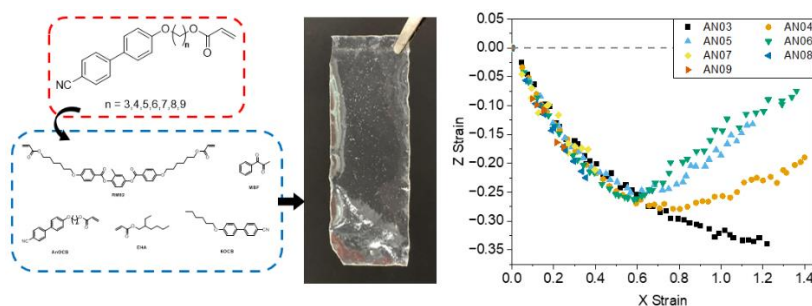


Figure 1. An example of the monomer modifications examined, in this case a series of cyanobiphenyl monomers of varying spacer lengths, and their impact on the auxetic response of the LCEs.

References

- [1] G. N. Greaves, A. L. Greer, R. S. Lakes, and T. Rouxel, *Nat. Mater.*, **10**, 823–837, (2011).
- [2] K. K. Saxena, R. Das, and E. P. Calius, *Adv. Eng. Mater.*, **18**, 1847–1870, (2016).
- [3] X. Ren, R. Das, P. Tran, T. D. Ngo, and Y. M. Xie, *Smart Mater. Struct.*, **27**, 23001, (2018).
- [4] D. Mistry, S. D. Connell, S. L. Mickthwaite, P. B. Morgan, J. H. Clamp, and H. F. Gleeson, *Nat. Commun.*, **9**, 5095, (2018).
- [5] Z. Wang, T. Raistrick, A. Street, M. Reynolds, Y. Liu, and H. F. Gleeson, *Materials*, **16**, 393, (2023).
- [6] C.T. Imrie, F.E. Karasz, G. S. Attard, *Macromolecules*, **26**, 3803-3810, (1993).
- [7] A. A. Craig and C. T. Imrie, *Macromolecules*, **28**, 3617–3624, (1995).
- [8] A. A. Craig and C. T. Imrie, *Polymer Vol.*, **38**, 4951-4957, (1997).

Surface instabilities of a half-space coated by a liquid crystal elastomer film

Yang Liu¹, Qianqian Ji², and Alain Goriely¹

1 Mathematical Institute, University of Oxford, Oxford, OX2 6GG, UK

2 Department of Mechanics, School of Mechanical Engineering, Tianjin University, Tianjin 300354, China

We consider the stability of a hyperelastic substrate coated by a liquid crystal elastomer film and subjected to compressive forces. In this problem, the liquid elastomer directors are free to evolve and need to be included in the incremental theory. Once that theory is established, we perform a standard bifurcation analysis. We assume that the initial directors are aligned either in the horizontal or in the vertical direction and obtain an exact bifurcation condition for surface wrinkling. We show that director reorientation both delay surface wrinkling and produce more wrinkles. In particular, our analysis unveils that the bilayer is more stable if the major-axis of liquid crystal molecules coincides with the alignment of the director. In the small wavenumber limit an asymptotic analysis is conducted to obtain analytical solutions for the critical stretch and the critical wavenumber, which can be relevant in applications.

The influence of UV exposure on polymer-stabilised liquid crystal blue phases

O. Niculescu*, O.J. Burtona, T.D. Wilkinson

Department of Engineering, University of Cambridge, Cambridge, CB3 0FA, UK

*on235@cam.ac.uk

The blue phase of liquid crystals is known for its fast, polarisation-independent phase modulating properties. Historically, it was only shown to be inherently stable within a very narrow temperature range, but this range was then improved and broadened using a polymer network [1]. In the process of obtaining blue phases, the polymer stabilisation occurs after growth, at temperature, upon exposure to UV radiation. The specific UV doses that the samples are subjected to have largely been set through empirical evidence.

This work intends to systematically analyse the impact of UV doses on polymer stabilisation, both in varying the dose and in varying the length of the exposure at the same dose, with the aim of facilitating the growth and stabilisation of larger platelets for enhanced homogeneity, and thus higher quality devices.

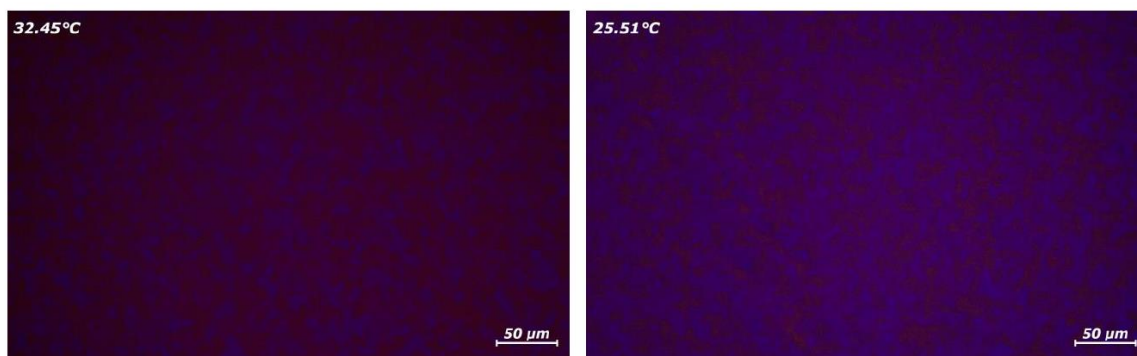


Figure 1. Liquid crystal blue phase sample under a polarising microscope, before (left) and after (right) polymerisation with 1 mW/cm² light for 37 minutes at 365 nm. The platelet quality is maintained.

This will be done, in the first instance, by utilising projection optics to modulate a gradient UV source and expose the sample for a given length of time, recording both its qualitative influence on the platelets in different areas of the cell, but also measuring the minimum temperature that the blue phase is still stable at. Thus, the full range between underexposure and overexposure will be studied. Moreover, once finding an appropriate UV dose, the exposure time will be varied within that dose. It is predicted that longer exposures facilitate the stabilisation of larger platelets [2], given the use of photoinitiator to aid with uniform UV penetration [3].

The results of this could bring to light a methodology for finding an ideal UV radiation dose for high throughput of devices in applications benefitting from larger, more uniform blue phase structures, approaching monodomains.

References

- [1] Kikuchi H., Yokota M., et al, *Nature Materials*. 1, 64–68, (2002).
- [2] Oton E., Netter E., et al, *Scientific Reports*. 7, 44575, (2017).
- [3] Liu Y., Xu S., et al, *Liquid Crystals*. 41:9, 1339-1344, (2014).

Numerical simulations for liquid crystal photonics

Urban Mur^{1,2}, Jaka Zaplotnik¹, Miha Ravnik^{1,3}

1. University of Ljubljana, Faculty of Mathematics and Physics, Ljubljana, Slovenia,

2. Department of Engineering Science, University of Oxford, Oxford, UK,

3 Josef Stefan Institute, Ljubljana, Slovenia

Liquid crystals (LCs) are distinct soft matter materials for use in photonics, because of their birefringence profile with spatially varying optical axis orientation and high susceptibility to external stimuli that can affect their internal structure. Numerical simulations are a useful tool to explain light behavior in such complex materials or to design desired optical properties. In this talk I will present the use of numerical simulations beyond standard light propagation, focusing on liquid crystal lasers in different settings, for example Cholestric Liquid Crystal (CLC) lasers or Fabry-Perot lasers with infiltrated liquid crystal structures. By employing combinations of widely used FDTD (Finite Difference Time Domain), FDFD (Finite Difference Frequency Domain) and semi-classical lasing equations, we can explain or predict and to an extent design the properties of output lasing light, like lasing frequencies, thresholds and polarisation and intensity profiles. Additionally, I will present how we can use a combination of FDTD method for light propagation and phenomenological Landau-de Gennes (LdG) free energy relaxation for liquid crystal reorientation to simulate mutual two way coupling between light and liquid crystal orientation.

All-atom simulations of CB6OIBeOn: a progress report

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

^aDepartment of Chemical Engineering, University of Manchester, Manchester M13 9PL, UK

^bDepartment of Chemistry, University of Durham, Durham DH13LE, UK

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

Abberley et al.¹ have reported fascinating phase behaviour for 4-[[4-{{6-[4-(4-cyanophenyl)phenyl]hexyl}oxy)phenyl]methylidene}amino]phenyl-4-alkoxy-benzoates (CB6OIBeOn), where n is the carbon number of the terminal alkyl chain. The molecular structure for $n = 6$ is shown in Figure 1. For $n \leq 6$, cooling yielded the phase sequence $I \rightarrow N \rightarrow N_{TB} \rightarrow \text{HexI} \rightarrow K$ (crystal) whereas for $n > 6$, the sequence was $I \rightarrow N \rightarrow \text{SmA} \rightarrow \text{SmA}_B \rightarrow \text{SmC}_{TB} \rightarrow \text{HexI} \rightarrow K$. The spontaneous formation of helical structures can render the phases as chirality.^{1,2} With the hope of casting lighter on the molecular organisation in these phases and the driving forces for their formation, we have embarked on a Molecular Dynamics simulation study. We have simulated 700 molecules, using the the General AMBER Force Field (GAFF) force field³, at a pressure of 1 bar.

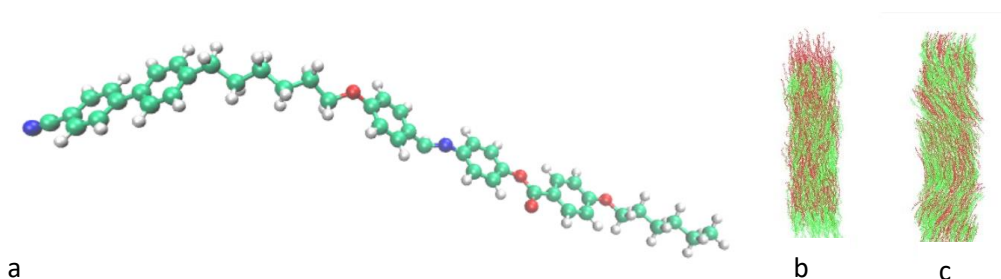


Figure 1. (a) Molecule structure of CB6OIBeO₆. Simulation snapshots of 700 CB6OIBeO₆: (b) shows a nematic phase at 520K and (c) shows a twist-bend nematic phase at 420K with different angle colouring between the long axis of molecules and y axis. The colouring reflects the ordering of the long axis of the molecules along the director.

To date we have observed the nematic phase N and the twist-bend nematic phase N_{TB} for $n = 6$, as shown in Figure 1. We are hopeful that on further cooling we shall observe the HexI phase and that studies on molecules for $n > 6$ will allow us to analyse the exotic smectic phases reported.

References

1. Abberley, J. P. et al. Helical smectic phases formed by achiral molecules. *Nat. Commun.* **9**, 228 (2018).
2. Yu, G. & Wilson, M. R. All-atom simulations of bent liquid crystal dimers: the twist-bend nematic phase and insights into conformational chirality. *Soft Matter* **18**, 3087–3096 (2022).
3. Wang, J., Wolf, R. M., Caldwell, J. W., Kollman, P. A. & Case, D. A. Development and testing of a general amber force field. *J. Comput. Chem.* **25**, 1157–1174 (2004).

Mathematical modelling of active fluids in a confined rectangular region

Joseph Kwajighu, Ijuptil, Mottram, Nigel J., Kowal Katarzyna N., Cousins, Joseph R. L.
School of Mathematics and Statistics, University of Glasgow, Glasgow G12 8QQ, UK

Active fluids are systems composed of self-driven units that consume and convert energy into directed motion. Motivated by possible applications in the design of sensors and for the general understanding of various biological processes, we present a 2D theoretical and computational study involving the mathematical modelling of active fluids confined between two parallel plates using an adapted form of the Ericksen-Leslie equations. We numerically solve the model, with imposed hybrid-aligned nematic (HAN) anchoring – where the average orientation of the self-driven units is parallel to the substrate at one plate and perpendicular to the substrate at the other. We characterise the range of flow profiles for varying magnitudes of the activity at a fixed channel width. For low-magnitude activities, the flow is characterised by a positive (negative) gradient of the velocity field in the left-hand (right-hand) regions. Further increasing the magnitude of the activities results in more localised flow. However, the system exhibits spatial fluctuation for sufficiently high magnitudes of activities, although there are no time-dependent oscillations in the system. For lower activities, we observed unidirectional flow, while for high activities we observed bidirectional flow characterised by an antisymmetric distorted state at the middle of the region. Our results lead to potential applications for designing sensors owing to the ability of small changes in the alignment of the self-driven units to ensure long-range effects in the orientation and flow of the active fluids.

Atomistic Simulations of Columnar Ordering of Triphenoxazoles - A New Class of Fluorescent Discotics

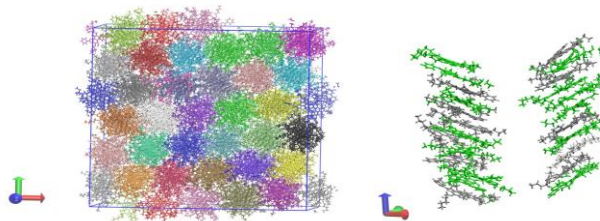
Arunkumar Bupathy,¹ Mark R. Wilson,² and **Dwaipayan Chakrabarti**¹

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

² Department of Chemistry, Durham University, Durham DH1 3LE, UK

*Corresponding author: d.chakrabarti@bham.ac.uk

Discotic liquid crystals in their columnar phase – a class of organic semiconductors¹ – are of particular interest for their potential opto-electronic applications.¹⁻³ The design of disc-like molecules, typically having an aromatic core with peripheral aliphatic chains, is crucial for controlling the photophysical and charge-transport properties of discotics, the latter being critically dependent on the molecular arrangements in the columnar phase.^{4,5} Atomistic simulations can provide valuable information for understanding molecular order in the columnar phase of discotic liquid crystals, but have proved challenging, often resulting in studies of thermal relaxation of pre-formed columnar phase,⁵⁻⁷ thus limiting detailed understanding of the growth of the columnar phase.⁸ Here, we report on the self-assembly of a tilted columnar phase for a representative mesogen from a series of triphenoxazoles – a class of recently synthesised fluorescent discotics⁹ – in all-atom detail (see the figure below).¹⁰ We demonstrate the spontaneous emergence of the columnar ordering, when cooled from the isotropic phase in atomistic simulations that extend into the μs regime. We characterise the columnar phase and investigate its growth across the phase transition. Our simulations show that the transition into the columnar phase is marked by the growth of a narrow peak in the cluster size distribution, concurrent with the coalignment of molecular stacks and positional ordering in the orthogonal directions.¹⁰ We analyse the local molecular arrangements in the columnar phase and discuss their implications for potential applications of this exciting class of compounds.



1. S. Sergeyev, W. Pisula and Y. H. Geerts, *Chem. Soc. Rev.*, 2007, **36**, 1902-1929.
2. B. R. Kaafarani, *Chem. Mater.*, **2011**, 23, 378-396.
3. T. Wöhrle *et al.* *Chem. Rev.*, 2016, **116**, 1139-1241.
4. X. Liu, Z. Xu and J. M. Cole, *J. Phys. Chem. C*, **2013**, 117, 16584-16595.
5. X. Feng *et al.* *Nat. Mater.*, **2009**, 8, 421-426.
6. D. Andrienko, V. Marcon and K. Kremer, *J. Chem. Phys.*, **2006**, 125, 124902.
7. S. Bag *et al.*, *J. Chem. Phys.*, **2015**, 143, 144505.
8. P. L. Cristinziano and F. Lelj, *J. Chem. Phys.*, **2007**, 127, 134506.
9. G. O'Callaghan *et al.* Manuscript in preparation.
10. A. Bupathy *et al.* Manuscript in preparation.

Liquid Crystals Droplets for Photonic Applications

Waqas Kamal, Steve J Elston, Stephen M. Morris, and Alfonso A Castrejón-Pita

Department of Engineering Science, University of Oxford, Oxford

Drop-on-demand (DoD) inkjet printing stands out as a precise, scalable, and cost-effective additive manufacturing technique that enables a plethora of materials to be deposited onto a range of different substrates. Over the past decade, there have been a number of reports that have showcased its potential of printing nematic and chiral nematic liquid crystals (LCs) for various applications such as sensors, printable lasers, and thermally-tunable microlenses. In this presentation, we highlight our recent research on inkjet printing of LCs and demonstrate a range of alternative photonics technologies fabricated using this manufacturing process. The presentation will begin by considering the conditions necessary to print LCs without jet break-up and satellite droplet formation before we show how to fabricate electrically tunable microlenses that exhibit bifocal tuning. Using homeotropic surfactants, plano-convex lenses with diameters ranging from 122 μm to 255 μm , resulting in focal lengths for red light ($\lambda = 633 \text{ nm}$) from 228 μm to 463 μm , respectively. Remarkably, these microlenses exhibit bifocal behavior under an electric field without altering the geometric shape of the lens. Furthermore, we present spatially patterned polymer dispersed LC films fabricated using this printing process and demonstrate new smart window technology featuring logos and images that can be made to disappear with the application of a voltage. The presentation concludes with a demonstration of colored reflector arrays along with an outlook to the future for this printing technique.

Stable and Metastable Director Fields in Printed Chiral Nematic Liquid Crystal Droplets

Alva C. J. Orr¹, Xuke Qiu¹, Thomas C. Sykes¹, Waqas Kamal¹, Steve J. Elston¹, Julia M. Yeomans², Stephen M. Morris¹, and Alfonso A. Castrejon-Pita¹

1. Department of Engineering Science, University of Oxford, Parks Road, Oxford, OX1 3PJ
2. Rudolf Peierls Centre for Theoretical Physics, University of Oxford, Parks Road, Oxford, OX1 3PU, UK

* alva.orr@eng.ox.ac.uk

The use of drop-on-demand printing confers various advantages over traditional manufacturing methods, for example the ability to digitally position droplets and manipulate their final size or composition. In this presentation, we investigate the optical properties and director profiles of drop-on-demand inkjet printed chiral nematic liquid crystal (CLC) droplets where we vary the dimensions of the droplet relative to the pitch, the distance over which the director field preferentially undergoes a full rotation. Such sessile droplets provide a unique confined geometry, with both a flat and curved homeotropic boundary condition within which the helices of the chiral nematic LC phase may form.

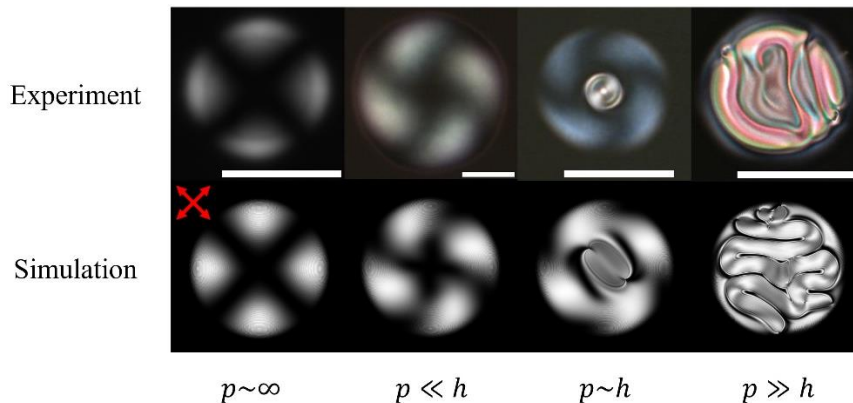


Figure 1: Experimental and simulated polarised optical microscopy images of chiral nematic liquid crystals onto homeotropically aligned substrates, with increasing chirality from left to right. Red double-headed arrows indicate the directions of the polariser axes, which are the same throughout all images. All scalebars are 100 μ m.

The printed droplets are found to exhibit three distinct regimes, depending on the ratio of droplet size to helix pitch. Weakly chiral droplets, where the pitch p is significantly longer than the droplet height h , exhibit a twisted vertical director field, but lack a distinct helical axis. However, in droplets where $h/p \sim 1$, a transitional regime develops in which the tight balance between the elastic energy and boundary conditions on the droplet leads to random drop-to-drop variation in the final director field. Even for identical printing conditions, some droplets develop the characteristics of a partial fingerprint texture, while others do not. The causes of this behaviour are investigated using free-energy minimisation techniques which account for the nematodynamics of the inkjet printing process. Careful consideration of the initial condition reveals these states to be metastable to each other and gives insights into how the final director configuration might be manipulated for manufacturing processes. The final regime, in which $h/p \gg 1$, tends towards the well-known 'fingerprint' texture, as the effects of the elastic energy dominate over the boundary conditions. Optical simulation techniques are used to compare the free-energy minimisation results with polarised optical microscopy images and excellent agreement is seen, as shown in Figure 1.

Long-pulse liquid crystal lasers: Redefining definitions of threshold

Calum M. Brown, Ieva Pakamoryte, **Philip J.W. Hands***

Institute for Integrated Micro & Nano Systems (IMNS), School of Engineering,
University of Edinburgh, Edinburgh, EH9 3FF

Corresponding author: Philip.Hands@ed.ac.uk

Photonic band-edge lasing from dye-doped chiral nematic liquid crystals (LCs) has been widely studied due to their ability to exhibit selectable wavelength lasing from a self-organised resonant microcavity. Recent advances in laser-diode pumping of LC lasers [1] provides new control mechanisms for lasing and enables new temporal studies of lasing output.

In this paper we first present our new laser-diode pumped LC laser platform [1,2], before revealing experimental results characterising the effect of pump pulse duration upon laser efficiency and threshold [3]. Longer pulse lengths have a detrimental effect on these parameters, however a detailed description and understanding of this requires a closer look at our definitions of lasing. Our experiments highlight the need for caution when attempting to make fair comparisons of laser performance across different experiments. To address this, we propose a new convention is adopted for the definition of threshold within organic lasers, in terms of peak power density.

By way of better understanding the results above, we also report on ongoing experimental and theoretical work on the temporal dynamics of photonic emission from LC lasers. These results are forming new hypotheses regarding the relative durations of stimulated and spontaneous emission processes (and hence the degree of coherence), and how these are affected by pump pulse duration. Our results provide new insights into the lasing process within dye-doped LCs (and other optically-pumped organic lasers), and may offer new mechanisms for designing bespoke laser sources for applications in medical imaging and holographic projection [4].

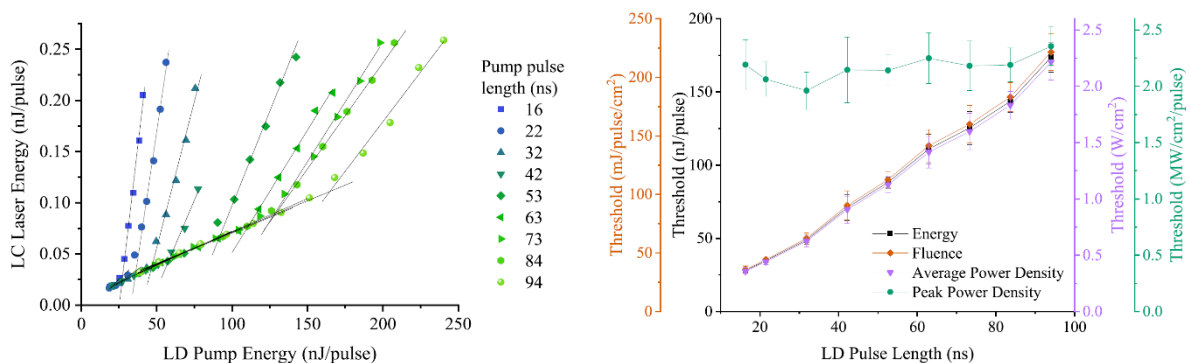


Fig. 1. Experimental data showing detrimental effects upon threshold and slope efficiency of increasing pump pulse length [3]. Note the pulse length invariance of threshold when plotted in terms of the peak power density (right-hand graph, green data points).

References

- [1] C.M. Brown, D.K.E. Dickinson, P.J.W. Hands, *Opt. Laser Tech.* 140, 107080, (2021).
- [2] C.M. Brown, D.K.E. Dickinson, P.J.W. Hands, *Proc. SPIE*, Vol. 11987, 1198703 (2022).
- [3] C.M. Brown, I. Pakamoryte, P.J.W. Hands, *Optics Letters*, 48 (18), 4873, (2023).
- [4] P.J.W. Hands, C.M. Brown, D.K.E. Dickinson, S.M. Morris, J.-D. Lin, *SID Digest*, 36-1 (2022)

The next generation of optical components for augmented and virtual reality headsets enabled by reactive mesogens

Peter Wyatt, Nina Podoliak, Benjamin Snow, Stephen Mulcahy, Owain Parri

Merck Performance Materials Ltd., 1 Venture Road, Southampton, SO16 7NP, UK

Merck is a vibrant science and technology company and global market leader in the liquid crystal display sector. At Merck Performance Materials based in Chilworth, Southampton, we are creating the next generation of reactive mesogen inspired optical materials to revolutionise future display technologies.

To continue in our position as the company behind the companies, we have made crucial developments and modifications to our reactive mesogen formulations to help shape the future of displays. These have been carefully formulated and designed with sustainability in mind, such as being PFAS free, using safer and green solvents, and can be polymerised with LED sources. These formulations will help create various optical components through a multi-layer coating approach in an R&D based setting, including:

- Super achromatic half and quarter waveplates,
- Achromatic lenses,
- Achromatic polarisation volume holograms for diffraction gratings and waveguides.

We envisage such components enabled by our formulations are crucial to the development of head-mounted displays, enabling both virtual and augmented reality systems to reduce in weight and form factor, while improving their efficiency and user related comfort such as an increased field-of-view. This talk will introduce these various optical components, some problems to be solved, and how our complex birefringent thin films work.

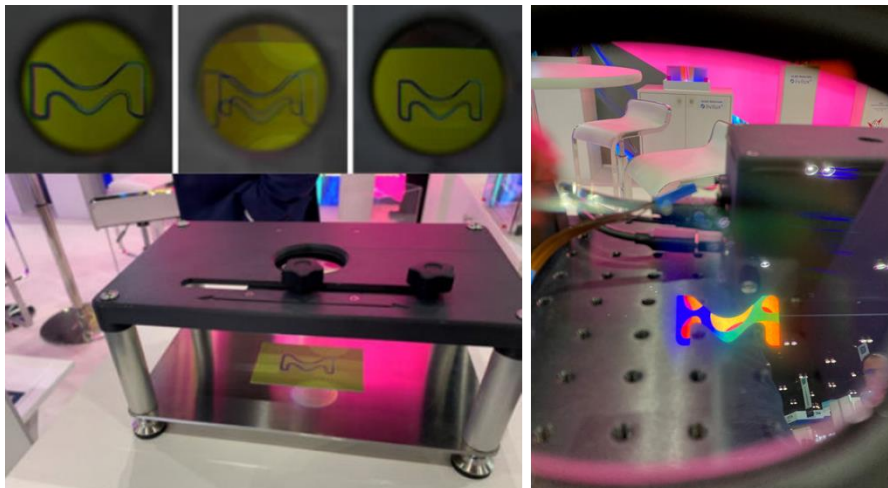


IMAGE: THE LENS (LEFT) AND WAVEGUIDE (RIGHT) DEMONSTRATORS SHOWN BY MERCK AT THE SID DISPLAY WEEK 2023 CONFERENCE. THE LENS DEMONSTRATOR SHOWS THAT THE MERCK LOGO CAN BE MAGNIFIED OR DEMAGNIFIED, WHILE THE WAVEGUIDE DEMONSTRATOR OVERLAYS THE MERCK LOGO INTO THE REAL WORLD.

Unusual applications: Liquid crystal sensors for ultrasonic displacement measurements

M. Turvey^{1*}, O. Trushkevych², D.J. McKnight³, K. Patel², R.S. Edwards¹

¹ *Department of Physics, University of Warwick, Coventry, CV4 7AL, UK*

² *School of Engineering, University of Warwick, Coventry, CV4 7AL, UK*

³ *Pictura Bio, Wood Centre for Innovation, Quarry Road, Oxford, OX3 8SB, UK*

* m.turvey@warwick.ac.uk

Visualising ultrasonic fields is important in the fields of non-destructive testing and structural health monitoring, as it can be used to see where defects form in structures/components and the progress of the defects over their lifetime. Laser vibrometry is the gold standard for wavefield visualisation, however, it is time consuming and expensive due to scanning requirements and the cost of equipment. A new method of visualising ultrasound propagation in structures, which could be done without the need for scanning, would help to improve safety.

Previously, polymer-dispersed liquid crystal (PDLC) films have been shown to allow for fast and low cost visualisation of ultrasonic fields. Thermochromic liquid crystal (TLC) films can be similarly used to map ultrasonic displacement. The ultrasonic field generates heat which can be absorbed in the sensor, changing the pitch of chiral nematic LC inside the film and therefore altering the wavelength of light reflected from it. Temperature values can be extracted using optical photography and true-colour image processing, which can be used as an approximation of comparative displacement due to ultrasound vibration; the temperature change corresponds to several factors including displacement, environment, and thermal conductivity of the sample.

TLC sensors have been tested in several visualisation tasks. First, distinct modal patterns at specific resonant frequencies of a flexural ultrasonic transducer were analysed. Secondly, the sensors have been used to visualise acoustic energy distribution in plates with straight and serrated edges, and in phononic crystal – type plate with periodic array of holes when excited by guided acoustic waves (Lamb waves). Finally, TLC films have been used to detect defects within a metal block; for example, for internal defect detection ultrasound is transmitted through a sample, and the areas where a defect is present block the ultrasound transmission, with the defect visible as a dark area on an otherwise colourful sensor. Examples of these applications are shown, with true-colour image processing used to analyse the wave behaviour.

Laser-written Tuneable Liquid Crystal Aberration Correctors

Alec Xu*, Camron Nourshargh, Chao He, Patrick Salter, Steve J. Elston, Martin J. Booth and Stephen M. Morris

Department of Engineering Science, University of Oxford, Oxford, UK

* alec.xu@eng.ox.ac.uk

In adaptive optics, image aberrations are frequently characterized by a series of orthogonal modes, such as Zernike polynomials. Generally, these modes are corrected using spatial light modulators, deformable mirrors, or fluidic transmissive devices. While these technologies are versatile, they can be expensive to integrate into the optical path, in terms of expertise, bulk and cost. They are often overspecified for applications where only a few modes need to be corrected.

However, direct laser writing offers a cost-effective alternative to these technologies. By mixing a liquid crystal (LC) with a monomer and photoinitiator, the LC mixture can then be selectively polymerized using a femtosecond laser that triggers polymerization through a two-photon absorption process. This process freezes director orientation of the polymerized bulk, allowing complex phase patterns to be imprinted into a single device, replicating many Zernike polynomials with easy and simple tunability.

As a demonstration of the versatility of the approach, we have recreated several separate Zernike polynomial modes, although this method could be adapted to far more modes. These devices are transparent and operated by a single AC electrode pair and can be continually tuned to a maximum total amplitude of more than 2π rad, and range in size from a diameter of 250 μm to 2000 μm . Analysis across the central axis of the phase tilt modulator verified that the phase error of the device was less than 0.25rad RMS, compared to an ideal tilt profile. These devices could be integrated into adaptive optics systems where space and cost are prohibitive and have potential impact in fields as diverse as astronomy, microscopy and ophthalmoscopy.

Photonic liquid crystal soft matter

Miha Ravnik^{1,2}

¹ *Faculty of Mathematics and Physics, University of Ljubljana, Ljubljana, Slovenia*

² *Josef Stefan Institute, Ljubljana, Slovenia*

Liquid crystals and structures of liquid crystals are capable of diverse control over the flow-of-light at the wavelength level, as well as below and above. In this talk, I will present recent results on the control over liquid crystal structures and emergent photonic phenomena. For structures, I will present the role of electric ions in liquid crystal doping and the role of chirality, such as in blue phases and skyrmions. For photonics, I will present the concept of pixelated photonic crystals, use of neural networks for optical reconstruction and/or prediction of liquid crystal fields and design of lasing modes by liquid crystal based resonators. More generally, the talk is aimed to emphasise selected possible exciting research directions in photonic liquid crystal soft matter.

Impact of Photoisomerization on the One-Dimensional and Three-Dimensional Photonic Structures of Liquid Crystals

Rajalaxmi Sahoo,* D. S. Shankar Rao, C. V. Yelamaggad, and S. Krishna Prasad

Centre for Nano and Soft Matter Sciences, Bengaluru, India

**Present address: School of Physics and Astronomy, University of Leeds, Leeds, UK*

Photonic Crystals (PCs) are dielectric structures with the periodicity of refractive index in one, two- and three-dimensions tailor-made for controlling or manipulating the propagation of electromagnetic waves of a specific wavelength. The range of wavelengths/frequencies of electromagnetic radiation forbidden for transmission through the PCs is known as photonic bandgap (PBG). Their ability to effectively manipulate the light shows potential applications in all-optical integrated circuits like optical filters, waveguides, low-threshold lasers, etc [1]. While various conventional fabrication techniques are routinely used to create PCs, it would be significantly advantageous if such periodic structures can be achieved just by self-assembly of molecules, a possibility for which liquid crystals (LCs) are ideal systems. Chiral nematic (Ch) and twist grain boundary smectic C* (TGBC*) liquid crystal phases are perfect examples of self-assembled structures exhibiting PBG in one- and three-dimensions, respectively [2]. The latter phase has a frustrated phase character and is analogous to the Abrikosov phase seen in type 2 superconductors.

The first part of the presentation describes the influence of guest monomeric photoactive dopant (azobenzene monomer) on the thermal and PBG properties of Ch and TGBC* phases [3]. The second part of the presentation demonstrates that by replacing the monomeric azobenzene molecule with a mesogenic dimer (in which the two azobenzene groups are separated by a flexible spacer), along with light the spacer and parity of the dimer effectively controls the characteristics of these phases [4, 5]. The photoisomerization effect is mapped using polarising optical microscope, laser diffraction, laser transmission and selective reflection studies. The experimental findings gain importance because the phototuning capability from three-dimensional to one-dimensional PBG structure is stable and reversible. Thus, the studies provide a convenient method to control the photonic character of these systems in all the three directions.

Topological data analysis: a roadmap to liquid crystal physics

Giampaolo D'Alessandro⁽¹⁾, Tristan Madeleine⁽¹⁾, Maria Van Rossem⁽²⁾, Oleksander Buchnev⁽²⁾, Ingrid Membrillo-Solis⁽¹⁾, Nina Podoliak⁽²⁾, Tetiana Orlova⁽²⁾, Jacek Bridzki⁽¹⁾ and Malgosia Kaczmarek⁽²⁾

⁽¹⁾ School of Mathematical Sciences, University of Southampton

⁽²⁾ School of Physics and Astronomy, University of Southampton

Topological data analysis (TDA) is a very “applied” branch of pure mathematics that provides robust tools for the analysis of spatially structured data. It has been used in a wide range of fields, from studying phase transitions in alloys to characterising images of diseased lungs and bones. In this presentation we will give a very brief hands-on introduction to these tools and illustrate their power using examples from disordered surfaces and liquid crystals. We will show how it is possible to classify the disorder of metasurfaces in order to obtain a requested optical response. We will also use it to trace the dynamics of suspensions of gold nanoparticles in liquid crystal capillaries and cells as they cross the isotropic to nematic phase transition point.

Design of new materials exhibiting polar & modulated liquid crystal phases

R. Walker

Department of Chemistry, University of Aberdeen, Aberdeen, AB24 3UE, UK

The simplest liquid crystal phase – the nematic phase – is nowadays ubiquitous in our daily lives, and its ability to switch on application of an electric field underpins much of the multi-billion-pound liquid crystal display industry. Current LCD technology is limited by the speed at which the nematic phase can ‘switch’ and for this reason – and of course scientific curiosity – we seek new liquid crystal phases with the possibility of transformative applications in displays and beyond. Two such ‘new’ phases, for which recent studies appear to show incredible potential, are also nematic in nature – the twist-bend nematic phase, NTB,[1] and the ferroelectric nematic phase, NF.[2] More recently, heliconical twist-bend smectic C (SmCTB) phases have also been discovered for liquid crystal dimers[3] and it appears that a range of variants of this phase, similar to the SmC* subphases observed for chiral molecules, are possible.

From a chemist’s perspective, understanding the molecular features influencing the formation and stabilisation of these new phases is of paramount importance, and allows for the design of new materials that have targeted properties. As such, recent work in Aberdeen has had the primary aim of enhancing our current understanding of these relationships in dimeric[4] and low-molar-mass liquid crystals,[5] through the synthesis and characterisation of a diverse range of materials.

References:

- [1] I Dozov. *Europhys. Lett.* 56, 247–253 (2001); M. Cestari et al., *Phys. Rev. E Stat. Nonlinear, Soft Matter Phys.* 84, 031704 (2011).
- [2] R.J. Mandle et al., *Phys. Chem. Chem. Phys.* 19, 11429–11435 (2017); H. Nishikawa et al., *Adv. Mater.* 29, 1–8 (2017).
- [3] D. Pocięcha et al., *Adv Mater.* 33, 2103288 (2021); A. Alshammari et al., *Soft Matter.* 18, 4679-4688 (2022).
- [4] R. Walker et al., *ChemPhysChem.*, 24, e202300105 (2023); A. Alshammari et al., *Liq Cryst.* Accepted. (2024).
- [5] E. Cruickshank et al., *ACS Omega*, 8, 36562-36568 (2023); E. Cruickshank et al., *Liq Cryst.*, DOI: 10.1080/02678292.2024.2304598 (2024).

The behaviour of high dipole (10.6-13.6 D) nematic mesogens based on a novel phenyl pyrimidine motif

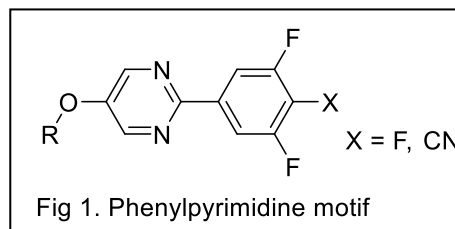
W. Jiang^{1#}, Yu. P. Panarin^{2,3#}, N. Yadav^{2#}, M. Sahai^{1,4}, Y. Tang⁵, X. Zeng⁵, O. E. Panarina², J. K. Vij², G. H. Mehl^{1*}

¹Dept of Chemistry, University of Hull, Hull HU6 7RX, UK;

²Dept. of Electronic & Electrical Engineering, Trinity College Dublin; University of Dublin, Dublin, Ireland;

³Dept. of Electrical & Electronic Engineering, TU Dublin, Dublin 7, Ireland; ⁴Dept. of Physics, Birla Institute of Technology & Science, India; ⁵Dept. of Materials Science & Engineering, University of Sheffield, Sheffield, S1 3JD, UK

Molecules with high terminal dipole moments have attracted intensive attention over the last few years, as materials of that type allowed a realisation of a long held concept of ferroelectricity in nematics.¹⁻⁴ Subsequently ferroelectric like properties detected in the S_{mA} phase⁵ and anti-ferroelectric behaviour⁶ has also been detected. Molecular architectures have been expanded also to polymers⁷. High dipoles architectures have been achieved by decorating aromatic ring systems with electron withdrawing substituents in such a manner that all main dipolar groups point broadly in the same direction. Typically -nitro, -fluoro or -cyano groups have been employed to achieve high terminal dipoles. In order to extend the chemical range of molecular architectures for molecules forming nematic phase behaviour we have explored the phenylpyrimidine motif shown in Fig. 1. It involves a strong directed dipole strengths whilst avoiding ionic species, and it has to the best of our knowledge has not been reported so far. By exploring the “R” groups used so far for reported ferro-nematic systems we are able obtain dipoles ranging between 10.6 -13.6 D, based on calculations using Gaussian at the B3LYP/ 3-21G+g(d,p) level of DFT. We will report here the results of the chemical synthesis and characterisation, as well as the structural analysis of the LC state using OPM, DSC and XRD methods as well as electro-optical studies and we will compare and discuss the results in the context of related materials.



References

- [1] M. Born, *Sitzungsber. Preuss. Akad. Wiss.*, **30**, 614, (1916); [2] X. Chen *et al.* *Proc. Natl. Acad. Sci. U. S. A.*, **117**, 14021, (2020); [3] R. Mandle *et al.* *Phys. Chem. Chem. Phys.*, **19**, 11429, (2017); [4] H. Nishikawa *et al.* *Adv. Mater.*, **29**, 1702354 (2017); [5] A. Manabe, *et al.* *Liq. Cryst.*, **48**, 1079, (2021); [6] X. Chen *et al.* *Proc. Natl. Acad. Sci. U. S. A.*, **119**, e2210062119, (2022); [7] X. Chen *et al.* *Proc. Natl. Acad. Sci. U. S. A.*, **120**, e2217150120, (2023); [7] S. Dai *et al.* *Macromolecules* **54**, 6045, (2021),

New Compounds Based on RM734 Which Exhibit the Ferroelectric Nematic Phase

Ewan Cruickshank^{1,2*}; Rebecca Walker², Grant J. Strachan³, Magdalena M. Majewska³, Damian Pocięcha³, Ewa Górecka³, John M. D. Storey², Corrie T. Imrie²

1. *School of Pharmacy and Life Sciences, Robert Gordon University, Aberdeen, AB10 7GJ, UK*
2. *Department of Chemistry, School of Natural and Computing Sciences, University of Aberdeen, Aberdeen, AB24 3UE, UK*
3. *See Abstract*

* e.cruickshank2@rgu.ac.uk

The least ordered liquid crystalline phase is the nematic phase, N. In the nematic phase, the centers of mass are distributed randomly, and the phase is non-polar. In 2017, there was the exciting discovery of a new type of nematic phase in two different compounds named: RM734 [1] and DIO [2], Figure 1. This polar phase was later termed the ferroelectric nematic phase, NF [3]. While RM734 and DIO, in terms of their chemical structures, appear to be somewhat different to each other, they do both share a large longitudinal dipole moment and some degree of lateral bulk. The polar ordering within the NF phase allows for the phase to be much more sensitive to electric fields than the nematic phase and thus the phase could be transformative in electro-optic technologies. There are currently around 150 different compounds reported in literature which have been shown to exhibit the NF phase [4-7] and it is crucial that the library of compounds showing this fascinating phase is expanded further. Here we report the transitional properties of a variety of three ring compounds which are based on the RM734 template and exhibit the ferroelectric nematic phase.

References

- [1] Mandle, R. J. et al. *Chem. - A Euro. J.* 23, 14554-14562 (2017).
- [2] Nishikawa. et al. *Adv. Mater.* 29, 1702354, (2017).
- [3] Chen, X. et al. *Proc. Natl. Acad. Sci. U.S.A.* 117, 14021–14031 (2020).
- [4] Mandle, R. J. *Soft Matter.* 18, 5014-5020 (2022).
- [5] Li, J. et al. *Giant*, 11, 100109, (2022).
- [6] Manabe, A. et al. *Liq. Cryst.* 48, 1079-1086, (2021).
- [7] Cruickshank, E. *ChemPlusChem.* e202300726 (2024)

Novel Longitudinal Polar Smectic Phases

J. Hobbs^{1*}, C. Gibb², D. Nikolova¹, T. Raistrick¹, H. F. Gleeson¹, R. Mandle^{1,2}

1. *School of Physics and Astronomy, University of Leeds, Leeds, UK, LS2 9JT*

2. *School of Chemistry, University of Leeds, Leeds, UK, LS2 9JT*

[*j.l.hobbs@leeds.ac.uk](mailto:j.l.hobbs@leeds.ac.uk)

In 2017, the ferroelectric counterpart (NF) to the classic paraelectric nematic phase (N) was discovered [1, 2], and since then the NF phase has become the hottest area in liquid crystal science currently. In the process of studying the NF phase in rod-like molecular systems, polar variants of the traditional smectic A (SmA) phase with the polarization vector parallel to the layer normal were discovered [3, 4] suggesting that polar variants of the traditionally apolar LC phases are experimentally possible.

In this talk it will be demonstrated that various longitudinally polar equivalents of both the paraelectric SmA and SmC phases are indeed formable. These phases show exciting properties such as ferroelectricity and anti-ferroelectricity as well as spontaneous chiral symmetry breaking resulting in a fluidic LC phase that selectively reflects visible light. We will also shed light onto the coupling of polar and LC transitions in LC materials through emergent phase behavior via mixture formulation whilst also demonstrating mixtures exhibiting room temperature NF phases.

References:

[1] R. J. Mandle, et al., *Phys. Chem. Chem. Phys.*, 19, 11429 (2017)

[2] H. Nishikawa, et al., *Adv. Mater.*, 29, 1702354 (2017)

[3] H. Kikuchi, et al., *Adv. Sci.*, 9, 2202048 (2022)

Alkylthio- Terminated Liquid Crystal Dimers and the Twist-Bend Smectic Phases

Abigail Pearson, John M.D. Storey, Corrie T. Imrie, Rebecca Walker

Department of Chemistry, School of Natural and Computing Sciences, University of Aberdeen, Aberdeen, UK

The twist-bend phases have been the source of great interest in recent years due to their interesting properties, and most notably as the first example of spontaneous mirror symmetry breaking in a fluidic state; a locally chiral phase formed from achiral molecules. First predicted by Meyer [1] and later by Dozov in 2001 [2], the twist-bend nematic (NTB) phase was first experimentally observed in 2007 in the liquid crystal dimer CB7CB [3]. Much more recently, the first examples of twist-bend smectic (SmCTB) behaviour have been observed [4], again in achiral bent dimers, such as the CT6O2Me.m series (Figure 1a)[5].

Since their discovery, much research has been dedicated to determining the structure-property relationships responsible for the formation and stability of the SmCTB phases, including changing the nature and structure of the mesogenic units, spacer length, and the addition of lateral or terminal groups. In the present work, we report two new series of liquid crystal dimers based on CT6O2Me.m, shown in Figure 1b: CT6O2Me.Sm and CT6O3Me.Sm. In both series, the terminal alkyl chain m has been replaced with an alkylthio chain Sm, to explore the effect of changing the nature of this terminal group on the phase behaviour, and the chain length $-SCmH_{2m+1}$ extended from $m = 1-18$. The position of the lateral methyl branch is also varied from the ortho- (2Me) to the meta- (3Me) position, and it appears that the position of this branch determines whether helical twist-bend phases or orthogonal smectic phases are formed in dimers with a short terminal chain.

References:

- [1] R. B. Meyer, in Les Houches Summer Sch. Theor. Physics, Mol. Fluids, 1976, 316–320.
- [2] I. Dozov, Europhys. Lett. 2001, 56, 247–253.
- [3] Cestari, M. et al. Phys. Rev. E, 2011, 84, 031704.
- [4] Abberley, J.P. et al. Nat. Commun., 9(1), 228; Walker, R. et al. (2019), Soft Matter, 15, pp. 3188–3197; Alshammari, A. et al. (2024) Liquid Crystals, Accepted manuscript.
- [5] Alshammari, A., Pearson, A. et al. (2024) Manuscript in preparation.

Locking-in States in a Nematic Pi cell

Adithya P. Nair, Nathan J. Spiller, Yihan Jin, Waqas Kamal, Zhiyu Xu, Steve J. Elston, and Stephen M. Morris

Department of Engineering Science, University of Oxford, Oxford, UK

Nematic liquid crystal (LC) Pi cells, constitute an important category of devices with potential in applications that demand a rapid switching process. Line singularities known as disclinations play an important role in the understanding of the topography and electro-optic phenomena in LC technologies and there are a number of different topological regimes in a Pi cell. Manipulating these singularities and defects in a precise and controlled way can unlock new functionality and electro-optic behaviour for a range of applications including tunable lasers and beam generators for optical communications.

This presentation explores the concept of manipulation of the domain regions in a nematic Pi cell through the control of nucleation and growth. We then propose potential applications based on this approach. Utilizing a combination of reactive mesogens and an optical projection system imprinting is achieved that forms spatial patterns of a polymer network in the pi-cell that locks- in various topological states. By modulating the voltage, distinct states with varying boundary conditions are generated, establishing a mechanism to impede nucleation and growth by polymerizing different topological regimes inside the LC device. This results in the creation of a fast shutter that switches between the twist state and the bend state with the ability to indefinitely remain in these states. Separately, bistability within the LC device is achieved by varying the temperature and reapplying a voltage in this locked-in regime, offering potential applications in the development of temperature-sensitive labels for transporting biological molecules, for example. Furthermore, by employing different combinations of topologies to lock in the director states, a bistable LC device responsive to voltage is created.

Investigating the influence of crosslinker concentrations on the phase templating of liquid crystal elastomers

Alanoud H. Al Suwaidan^{1*}, Devesh Mistry¹, Richard J. Mandle^{1,2} and Mamatha Nagaraj¹

1. *School of Physics and Astronomy, University of Leeds, U.K*

2. *School of Chemistry, University of Leeds, U.K*

* ml19aas@leeds.ac.uk

Polymer templating has been an attractive field as ‘templating’ can be used to control the structure and the morphology of the polymer. Templated polymers are invaluable in producing complex nanostructured materials with enhanced functional properties and behaviors[1]. Liquid crystals (LC) have been utilized as a templating medium to create LC polymer networks, which show stimulus-response and enhanced functionality [2, 3]. Liquid crystal elastomers (LCEs) are a new class of polymeric materials that combines the properties of LC anisotropy and rubber elasticity, resulting in stimuli-responsive properties and unique mechanical behaviors.

Cross-linkers play an important role in mechanical and optical properties of LCEs and also in elastomer templated networks. Studying the influence of synthesis and crosslinker concentration on LC order and phase templating allows for understanding the properties and behavior of LCEs and decoupling the effects of composition from structure and order[5]. In this work, the influence of crosslinker concentrations on phase templating of LCEs has been investigated. Isotropic LCEs were produced by diluting the monomers with a range of solvents, while nematic LCEs were created by adding a nonreactive mesogen 6OCB. A combination of polarising optical microscopy and differential scanning calorimetry have been used to measure the phase transition temperatures of the mixtures. Isotropic LCE samples showed an increase in TNI and Tg by increasing crosslinker concentration and at a value of the crosslinker ~6 mol% , the isotropic phase was stabilized and persisted following the drying of polymerised materials. Moreover, the addition of 6OCB and ~6 mol% crosslinker resulted in the formation of isotropic LCE at 60°C polymerisation, while monomdomain nematic LCE was produced at 22°C polymerisation. By construct, at lower crosslinker concentrations, LCEs that polymerised in the precursor’s isotropic phase exhibited a transition to a polydomain nematic state at room temperature upon 6OCB removal. The ability of templating phases with ~6 mol% of crosslinker was further demonstrated by adding the chiral dopant CB15 to the nematic precursor. The resultant LCE exhibited an oily streak texture, consistent with the chiral nematic phase.

References

1. Clapper, J.D. et al. *Chem. of Materials*. 2008, 20(3), pp.768-781.
2. Nagaraj, M. *Crystals*. 2020, 10, p.648.
3. van der Asdonk, P., Kouwer, P.H.J. *Chem. Soc. Rev.* 2017, 46(19), pp.5935-5949.
4. Mistry, D. et al. *Macromolecules*. 2020, 53(10), pp.3709-3718.
5. Traugutt, N.A. et al. *Soft Matter*. 2017, 13(39), pp.7013-7025.

Optical Skyrmions through the lens of Cohomology

An Aloysius Wang, Steve J. Elston, Stephen M. Morris, and Chao He
Department of Engineering Science, University of Oxford, Oxford, UK

An exciting application of liquid crystal (LC) technology that has emerged in recent years is in the generation of structured polarization fields such as the optical Skyrmion. As a topologically protected state, the optical Skyrmion holds the potential to be a robust way of encoding information into the electromagnetic field, and the efficient synthesis of Skyrmions using LC devices has recently enabled the experimental verification of the topological robustness of the optical Skyrmion. In this presentation, we discuss the mathematical theory behind optical Skyrmions and the role in which LC spatial light modulators have played in pushing the boundaries of topological structured fields.

Laser Written Diffraction Gratings and On-chip Optical Waveguides

Bohan Chen, Peng Xie, Patrick S. Salter, Zimo Zhao, Camron Nourshargh, Mengmeng Li, Linpei Xue, Xuke Qiu, Chao He, Martin J. Booth, Steve J. Elston, Stephen M. Morris

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

Two-photon direct laser writing (TPP-DLW) is an advanced fabrication technique enabling precise and intricate three-dimensional nanostructure fabrication. TPP-DLW in polymerizable liquid crystals (LC) facilitates the development of innovative electrically switchable and mechanically flexible microstructures, with potential applications in augmented reality (AR)/virtual reality (VR) displays, optical beam steering, integrated optics, and more. This presentation will present a strategy for fabricating novel tunable diffraction gratings and optical waveguides that can either be electrically switchable or mechanically tunable using a combination of laser writing and ultraviolet (UV) polymerization. For the diffraction gratings, the formation of periodic polymer networks lock-in the LC director via DLW resulting in alternating regions of high and low refractive indices. Before UV illumination, the gratings can be switched on and off by adjusting the applied voltage. Upon exposure to UV light, the LC director in the nonwritten regions adopts a different alignment and a periodic variation in the refractive index is fixed in the LC gel. The far-field diffraction pattern can be tuned by mechanically stretching the flexible film. Similarly, for the LC waveguides, these can be switched between on and off states by altering the external electric field. Following UV polymerization, the waveguiding properties on flexible free-standing film are demonstrated.

Reconfigurable Optically Transparent Patch Antenna Using Nematic Liquid Crystals

Bradley C. Mee, Waqas Kamal, Stephen M. Morris, Steve J. Elston, Justin P. Coon

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

Design, simulation, fabrication and measurement of a patch antenna that is transparent in the optical domain and exhibits a controllable frequency response using a nematic liquid crystal (LC), is reported here. The antenna is fabricated by etching indium tin oxide (ITO) coated glass to produce the antenna feed and radiating patch, with the LC mixture E7 inkjet printed directly onto the patch, with a second ITO coated glass cell employed to sandwich the LC, and act as the antenna's ground plane. A continuously tunable frequency response is achieved by controlling the dielectric permittivity of the E7, via an externally applied electric field between the patch and ground plane. Measurements of the antenna show a transmittance through the two glass slides and LC 65 μm thick of 55% between 400nm – 800 nm wavelengths, antenna efficiency of 99% at 6.9 GHz, and a continuously reconfigurable range of 100 MHz.

Laser Written Liquid Crystal Optical Vortex Beam Generators

Camron Nourshargh, Alec Xu, Patrick S. Salter, Martin J. Booth, Steve J. Elston, and Stephen M. Morris

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

We present a liquid crystal (LC) optical vortex (OV) generator that is tuneable in both wavelength and OAM state. Two photon polymerisation is an additive manufacturing technique that can be used to selectively polymerise a photoresist. Here, it is used to write 3D polymer structures into single electrode pair LC devices. In this way, the director field of the polymerised LC is locked in place, while the non-polymerised LC is still electrically addressable, yielding phase plates that are continuously tuneable post fabrication. The structure demonstrated here are designed to convert linearly polarised light with a wavelength of 633 nm into an optical vortex whose OAM can be tuned from 0-2. Initial analysis of the device is performed using polarisation optical microscopy (POM). The performance of the device is characterised using a series of laser transmission measurements, including far-field and interference imaging. The performance of the laser at a range of wavelengths from 520nm to 780 nm is also demonstrated. A finite difference method is employed to simulate the director profile of the LC device before and after the fabrication process and is used to confirm the POM images and gain an understanding of the effect of the laser writing process on the 'non-polymerised' LC. The transmission measurements are compared with a simulation of those produced by an ideal OV to demonstrate the performance of the device.

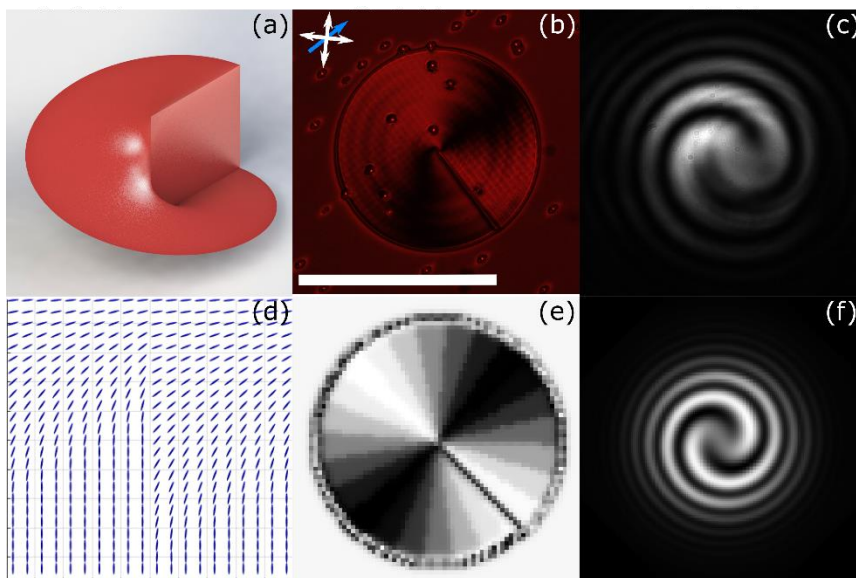


Figure 1: (a) Cad model of laser written structure, (b) POM image of LC OV generator, (c) spherical interference image produced by LC OV generator under laser illumination, (d) simulated director field laser written structure, (e) simulated POM image of device, (f) simulated spherical interference pattern.

Phase Front Elements

Dezhi Shen, Antoni Wojcik, David R. Selviah, F. Anibal Fernandez*

Department of Electronic & Electrical Engineering, University College London, Torrington Place, London WC1E 7JE UK

*a.fernandez@ucl.ac.uk

Liquid Crystal on Silicon (LCOS) panels combine the optical processing capability of liquid crystals and the high performance electronics of CMOS. They have been traditionally designed for amplitude modulation projection displays but are now most commonly used for phase modulation applications, SLMs and holograms, with the assumption of a flat-top element function (constant amplitude and phase over each pixel) to construct the desired far-field (diffracted) response. A primary interest for these applications is high resolution and this has meant a continuous reduction of pixel size (currently of the order of $4\ \mu\text{m}$), which in turn results in high inter-pixel crosstalk and departure from the pixel's flat response. Furthermore, LC defects, that inevitably appear, now occupy a proportionally much larger part of the pixel area and drastically deteriorate the response and efficiency.

Here, we explore a drastic size reduction (as small as $2\ \mu\text{m}$). For this, we propose a new pixel architecture which no longer implements the uniform phase and amplitude profiles at each pixel. LCOS devices generally requires Computer-Generated Holography (CGH) for display. However, conventional CGH algorithms assume a uniform amplitude and phase response of a pixel. Consequently, in this work, we also modify the conventional CGH algorithms to accommodate the new LCOS response.

The liquid crystal modelling is based on the Landau-DeGennes formalism, taking into account order variations and is designed for the study of structures containing small features and LC defects where diffractive effects are likely to occur [3, 4]. The electromagnetic modelling, designed to model accurately these diffractive effects, is a finite difference in the frequency domain (FDFD) solution for the electric field and uses the tensor permittivity found by the LC modelling [5]. An efficient preconditioning scheme is used that allows the fast convergence of large structures.

Stokes parameters and polarization properties of band-edge liquid crystal lasers

Guanxiong Zhang, Chao He, Steve J. Elston, Stephen M. Morris*

Department of Engineering Science, University of Oxford, Oxford, UK

In this paper, we demonstrated the Stokes parameters of band-edge liquid crystal lasers and characterized their polarization states as not perfect, but close to circular with the same chirality as the handedness of the liquid crystal helices. Our measurement approach involved utilizing an imaging Stokes polarimeter with a rotated quarter waveplate, allowing for a detailed indication of Stokes parameters for each pixel across the laser wavefront. To mitigate measurement noise arising from pulse fluctuation in liquid crystal lasers, we implemented calibration techniques and appropriate averaging methods for each quarter waveplate orientation. Our investigation revealed that factors of excitation fluence from the pump source, cell thickness, and liquid crystal alignment can affect the degree of polarization and circularity of the laser emission. This polarization study of band-edge liquid crystal lasers provides an explanation of the non-circular polarization that could potentially support applications involving the control of polarization in liquid crystal lasers.

Tunable Waveguides with Liquid Crystals

Ji Qin, Zhikai Pong, Zimo Zhao, Yifei Ma, An Wang, Xuke Qiu, Martin J. Booth, Patrick S. Salter, Steve J. Elston, Stephen M. Morris, and Chao He

Department of Engineering Science, University of Oxford, Parks Road, Oxford

Liquid crystals (LC) play an important role in a wide variety of applications due to their birefringence, which can manipulate properties of light such as phase, intensity, and polarization. In this work, we design tunable LC-based optical devices and plan to fabricate them in conjunction with the direct laser writing (DLW) technique. LC layers, which can be switched by applying external electric fields, are integrated into DLW-based optical waveguides, in order to achieve high-speed beam modulation with controllable optical parameters. Such a unique structure paves the way for next-generation optical signal processing and computing devices.

Printed Liquid Crystal Droplets for Tunable Microlenses

Jinge Guo, Waqas Kamal, Mengmeng Li, Xuke Qiu, Alfonso A. Castrejon-Pita, Steve J. Elston, Stephen M. Morris

Department of Engineering Science, University of Oxford, Oxford

This poster presentation focuses on the physical and optical properties of positive and negative dielectric anisotropy liquid crystal (LC) droplets. Inkjet printing was used to print droplets with 100 μm diameter onto glass substrates with a homeotropic alignment layer. With the application of an electric field orthogonal to the plane of the glass substrate, we observed that for positive dielectric anisotropy LC droplets, the birefringence decreased with an increase in the voltage. In contrast, for negative dielectric anisotropy LC droplets, the birefringence increased as a result of the alignment of the director perpendicular to the direction of the applied electric field. However, we also observed that for negative dielectric anisotropy LC droplets the application of a high voltage resulted in the formation of a spiral structure at the centre of the droplets. Simulations were conducted to understand the formation of this spiral structure.

Enhancing Light-driven Polymer Stabilized Liquid Crystal Smart Devices

Junseok Ma^{1,2}, Seungwon Oh³, Jinyoung Choi¹, Hyunwoo Oh¹, Stephen M. Morris^{2*}, and Wooksung Kim^{1*}

1. *Department of Electrical Electronics Engineering, POSTECH, Pohang 37673, Republic of Korea*
2. *Department of Engineering Science Parks Road, Oxford OX1 3PJ, UK*
3. *Department of Electrical Information Communication Engineering, Kangwon National University, Republic of Korea*

The utilization of light as a clean and renewable energy source holds great promise for driving reconfigurable smart devices based on liquid crystals (LCs), such as smart windows and smart antennas, obviating the need for complex electronic driving schemes and electrode architectures. The incorporation of push-pull azobenzene with LCs has become a prevalent approach for designing light-responsive smart windows due to its rapid response characteristics. Nonetheless, the operational range of LCs/Azo composites is typically constrained by temperature considerations, particularly within room temperature or colder environments, impeding device operation in these conditions. To address this limitation, we have studied a hybrid modelling methodology that combines the implementation of a ultraviolet (UV) absorber with push-pull azobenzene compounds.

In this presentation, we describe a new way of modelling devices that include push-pull azobenzene compounds, UV absorption, and polymer-stabilized LCs (PSLCs). Using polymer networks can be an effective solution for substantially reducing relaxation times and the presence of a UV absorber can enable the modulation of the operational temperature range, enabling effective device operation at or below room temperature levels. We have studied the complex effects of such materials on modulating the operating temperature range and report how the UV absorber decreases the minimum operating temperature through heat irradiation. However, a side effect is that it decreases the maximum operating temperature thereby reducing the total operating temperature range. This study highlights the significance of considering the operating temperature range when designing smart devices that utilize azobenzene. By experimenting with different dopants, we aimed to expand the range of temperatures at which these devices can effectively operate, addressing a crucial limitation in their performance.

Time-Dependent Phase Modulation in Liquid Crystal Photonic Devices

Linpei Xue, Steve J. Elston, Stephen M. Morris

Department of Engineering Science, University of Oxford, Oxford, UK

Spatial light modulators (SLMs) serve as indispensable tools in modern optics and imaging applications, enabling dynamic control over the phase, amplitude, and polarization of light. Analogue full 2π phase modulation, fast response speed, low operation voltage as well as polarization independent are highly demanding in next-generation applications. In this presentation, we investigate the optical phase modulation potential of different nematic liquid crystal (LC) devices including the pi-cell operating in the so-called symmetric H (Hs) state and super twisted nematic (STN) device operating in the twisted Hs state. We have developed two experimental setups based on phase-shifting interferometry, employing Michelson interferometer and Mach-Zehnder interferometer, separately. Simulations are conducted using Ericksen-Leslie continuum theory, complemented by Jones calculus for the twist LCs structure. The measured results show great consistency with simulated results, validating the efficacy of our initial modulator design objectives.

The ferroelectric nematic behaviour of DIO analogues containing a heteroaromatic moiety

Marijus Juodka^{*}, Rebecca Walker, Corrie C. Imrie, John M.D. Storey

Department of Chemistry, School of Natural and Computing Sciences, University of Aberdeen, Aberdeen, AB24 3UE

In 2017, Nishikawa et al. reported a new liquid crystalline material called DIO (Fig. 1) which on cooling displayed three distinct mesophases.[1] During the initial investigation, the lowest temperature phase displayed a large transition enthalpy, indicating appreciable reordering of the molecules, accompanied by highly birefringent texture, observed using polarised optical microscopy.[1] Dielectric measurements revealed a spontaneous polarization phenomenon and its remarkable ferroelectric character, confirming Born's hypothesis on the existence of ferroelectric fluids if the dipolar interactions are strong enough to overcome thermal fluctuations.[1,2] The same year, RM230 (Fig. 1), another material exhibiting such a mesophase with high polar ordering was discovered, giving rise to a new chapter of liquid crystal studies: the ferroelectric nematic phase (NF).[3]

Since then, many theories on the formation of the NF phase were reported and, with the help of computational and organic chemistry, some prerequisites for the molecular structure to encourage the formation of the highly polar mesophase were determined.[4–6] One area which has been explored to a lesser extent is the effect of including a heteroaromatic structural element in the DIO structure. In the present work, we have synthesised a series of DIO analogues with a fluorinated pyridine moiety (Fig. 2), and analysed their phase behaviour.

Printed Liquid Crystal Droplets for Optical Vortex Beam Generation

Mengmeng Li, Steve J. Elston, Chao He, Xuke Qiu, Alfonso A. Castrejón-Pita, and Stephen M. Morris

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

Inkjet printing is employed across various fields, including biosensing, flexible electronics and more. The process of inkjet printing streamlines manufacturing and reduces costs and time by allowing for precise, customizable, and scalable production of materials on various substrates, with the added benefits of energy efficiency and minimal waste. Using inkjet printing to deposit liquid crystal (LC) mixtures offers an alternative fabrication technique in the field of optical components that can pave the way towards new functionality and applications. In this presentation we use printed LC droplets to generate optical vortex beams, which can be activated and deactivated by manipulating the amplitude of the electric field. Both simulations and experiments were carried out to determine the optical characteristics of the printed LC devices and the resulting far-field patterns for different input polarizations of light. We show that the LC droplet generator can produce both vortex beams and vector fields, the choice of which is determined by the polarization of the input light.

Spherical Microparticles Dynamics in Anisotropic Fluids Under Electric Fields

Mona Alsubaie and Ingo Dierking

Department of Physics and Astronomy, University of Manchester, Manchester, M13 9PL, UK

Liquid crystals (LCs) have a wide variety of applications, propelling them to the forefront of electro-optics and displays. In recent applications the behavior of liquid crystals relies on particles suspended within them. Yet, the particle behaviour and distribution can be significantly influenced by the application of an electric field. As a result, particles dispersed in the liquid crystal experience forces that can induce motion, change their translational direction, and even spatial organization[1]. Polarizing microscopy enables the examination of alignment quality and facilitates the identification of the electric field-frequency stability regimes where particular particle behaviors are observable [2].

To initially validate results, we focused on analyzing spherical silica particles suspended in nematic liquid crystals, where the motions are characterised via video analysis and were circular, linear, and random motion can be observed. The interplay between various length scales in chiral nematics, such as pitch length, particle diameter, and cell thickness, appears to significantly influence the observed behavior. For example, if the particle size is comparable to the pitch length, it can disrupt the LC structure and affect the motion. The data suggest that it's possible to achieve a degree of control over microparticle movements, which corroborates and expands upon findings from previous preliminary studies[3].

Further investigations will enable a comparative analysis of particles with diverse shapes, including rod-shaped particles, bent-shaped particles and eventually randomly shaped particles. It is anticipated to extend the observations to nanoparticles and nanoparticle aggregates of differently shaped constituents.

References

1. Dierking, I., G. Biddulph, and K. Matthews, *Electromigration of microspheres in nematic liquid crystals*. Physical Review E, 2006. **73**(1): p. 011702.
2. Lazo, I. and O.D. Lavrentovich, *Liquid-crystal-enabled electrophoresis of spheres in a nematic medium with negative dielectric anisotropy*. Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences, 2013. **371**(1988): p. 20120255.
3. Oh, J., H.F. Gleeson, and I. Dierking, *Electric-field-induced transport of microspheres in the isotropic and chiral nematic phase of liquid crystals*. Physical Review E, 2017. **95**(2): p. 022703.

A Liquid Crystal Active Screen for RGB Laser Speckle Reduction

Nathan P. Spiller *, Yihan Jin, Steve J. Elston, and Stephen M. Morris

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

This study presents a comprehensive investigation on the development and performance of novel liquid crystal (LC) active screen speckle reducers tailored for RGB (red, green, blue) illumination sources.

Lasers are highly desirable for imaging and display applications due to their directionality, intensity, and wide colour gamut. However, the inherent coherence of laser light introduces a phenomenon known as speckle. Resulting from interference effects, speckle is a spatially distributed granular distortion superimposed on the desired image. To address this issue, we propose innovative devices, based on short-pitch chiral nematic LCs, that are compact, lightweight, inexpensive and contain no moving components.

These devices act as volume-scattering active screens and can simultaneously reduce the speckle distortion across a range of visible wavelengths. By adjusting the driving electric field amplitude and frequency for these devices different ‘modes’ of operation can be selected depending on the desired level of speckle reduction. Experimental results demonstrate a significant reduction in speckle visibility while maintaining the desired colour performance. Detailed characterisation, including speckle contrast reduction, is presented. Additionally, the advantages of the active screen approach are emphasised by direct comparison to transmissive LC speckle reducers. Some of the best-performing devices can reduce speckle close to the imperceptible limit for the human eye. As such the developed LC speckle reducers offer promising solutions to mitigate speckle in RGB laser illumination projectors. These advancements have the potential to enhance various laser-based projectors, enabling high-quality, speckle-free imagery.

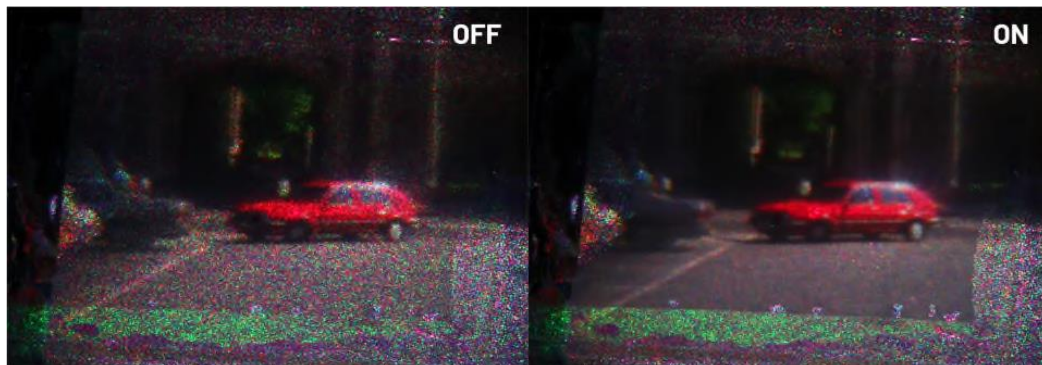


Figure 1: RGB Demonstration of the LC active screen speckle reducer. Left: No electric field applied to the LC device. Right: Optimum electric field conditions applied to the LC device for the lowest visible speckle contrast.

Flexoelectric-Liquid Crystal Diffraction Gratings for Beam Steering Technology

Qihao Han, Waqas Kamal, Stephen M. Morris, and Steve J. Elston,

*Department of Engineering Science, University of Oxford, Parks Road, Oxford, OX1 3PJ,
United Kingdom*

qihao.han@stx.ox.ac.uk

This poster presents an approach to optical beam steering using flexoelectric coupling in nematic liquid crystals (LC) that results in the formation of a field-driven diffraction grating. The presentation considers both theoretical modelling and experimental analysis. A novel nonlinear analytical model is constructed that incorporates dielectric coupling for a more accurate set of flexoelectric steady-state equations. Through numerical simulations, this model enables a visualization of the LC director behaviour under both flexoelectric and dielectric coupling. In parallel, a mixture was developed using nematic LC mixtures MLC-6882 and BL006, and the LC dimer CB7CB. This mixture exhibits a nematic phase at room temperature and facilitates real-time control of the diffraction angle and intensity into different diffraction orders by adjusting the magnitude of the DC electric field. Simulation results were found to closely align with experimental data, demonstrating the reliability and accuracy of the proposed model.

An alternative set of polarisation metrics for information analysis

Runchen Zhang, Xuke Qiu, Zimo Zhao, Yifei Ma, Steve J. Elston, Stephen M. Morris, and Chao He

Department of Engineering Science, University of Oxford, Oxford, UK

The Mueller Matrix Polar Decomposition (MMPD) method enables the decomposition of a Mueller matrix into a predetermined sequence of optical components—a diattenuator, retarder, and depolarizer—thereby determining their specific properties. Retarders serve important roles in medical applications such as the characterization of the fibrosis process in cancer detection. For the retarder segment, it is customary to further break it down into a combination of circular and linear retarder. This process characterizes a general retarder by three parameters: circular retardance, linear retardance, and linear axis orientation. However, this set of parameters significantly depends on the order of the circular and linear retarder and this approach can lead to misunderstandings when interpreting general elliptical retarders.

In this work, we examine the influence of the alignment sequence on the decomposition outcomes of the retarder sub-matrix, and then we introduce an alternative set of parameters for accurately characterizing a general elliptical retarder and validate its application across archaeological artefacts, biomedical specimens, and liquid crystal samples. This work paves the way to a better understanding of the polarization characteristics of biomedical and archaeological samples.

Simulations of liquid crystal tactoids

Sarangi Krishna

Materials and Engineering Research Institute, Sheffield Hallam University

Tactoids are fluid droplets made from nematic liquid crystalline materials set in an isotropic background fluid. The equilibrium shape of these droplets is a result of the complex interaction of the nematic elasticity, the surface tension and anchoring properties (alignment of the liquid crystal molecules at droplet surface). Depending on these contributions droplets can appear anywhere from spherical to highly elongated.

In this work we have developed a simulation tool to accurately model tactoid droplet shapes in 2D and 3D. The simulations involve minimisations of appropriate free energies and an ability to handle boundary shape changes. In the work here we numerically study the shape of tactoid and director field structure by focusing on the competing energies of surface tension, anchoring strength and elasticity. These energies are minimised using the Morpho software.

The initial mesh is initialised with a homogenous director field. The one elastic constant approximation is used in which $K_1=K_2=K_3=K=1$ and anchoring strength is varied in the range 0 to 10, as per Prinsen paper [1]. The tactoid droplets showed elongated shape at higher anchoring strength and came out to be spherical at the lowest or zero anchoring. Using the Morpho simulation tool, we could able to calculate aspect-ratio of tactoids and compare them along with the published results from Prinsen and Vanderschoot paper. Similarly total free energy contributions were calculated and plotted against anchoring energy. To advance to the 3D simulation of tactoids the 2D initial mesh of the previous section was replaced by a 3-dimensional mesh. Both our results of aspect-ratio and total energy are finding excellent agreement and validating the simulation methods adopted.

Future steps will aim to develop the model to simulate liquid crystal elastomers - materials that exhibit interesting responses in response to external stimulus.

References:

1. Prinsen, P., & Van Der Schoot, P. (2003). Shape and director-field transformation of tactoids. *Physical Review E*, 68(2), 021701.

Complex Structured Light Generation using Printed Liquid Crystal Droplets

Xuke Qiu, Runchen Zhang, Mengmeng Li, Zimo Zhao, Yifei Ma, Steve J. Elston, Alfonso A. Castrejón-Pita, Stephen M. Morris, and Chao He

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

We report a novel study on structured light generation using a high-precision ink-jet printing method to place liquid crystal (LC) droplets on specially prepared glass substrates. Our technique refines the internal structure of the LC within the droplets by applying homotropic and planar alignment conditions, which consequently shape the emerging light into various complex optical field configurations. The study details the creation of not only full Poincaré beams with orbital angular momentum but also introduces azimuthal/radial polarization and optical singularities. These structured light fields have implications for a multitude of applications including high-density data storage, optical communication, and microscopy. The methodology signifies a significant improvement over current structured light techniques, offering a simple, adjustable, and highly efficient production process for the next generation of photonic devices.

Electromagnetic Modeling of Liquid Crystal Based Reconfigurable Intelligent Surfaces in Terahertz Communications

Zhi Chai, Zimo Zhao, Steve J Elston, Stephen M. Morris, and Justin P. Coon

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

In terahertz (THz) communications, limited coverage due to signal attenuation and absorption is a critical issue. Reconfigurable intelligent surface (RIS) technology is a promising technique that can solve this problem owing to its ability to optimize the propagation environment. In this paper, we propose a novel RIS structure that uses a nematic liquid crystal (LC) as the tunable element to continuously control the impinging wave's phase. We propose a method to approximate the reflected phase shift for a single LC reflecting element. In addition, an LC element with the nematic mixture E7 as the LC material is fabricated, and measurements are conducted at THz frequencies using TeraSmart.

By comparing the numerical results obtained through the approximation with the measured results from the experiment, we verify the accuracy of the approximation and the continuous phase shift ability of a single LC-reflecting element. Next, we evaluate the performance of the LC-based RIS (LC-RIS) as a passive beamformer that works in the electrically small regime with conventional RISs (both 1-bit and 2-bit) as benchmarks. Directivity is used as the performance metric. The performance variation of the LC-RIS with respect to the thickness of the LC reflecting element, the incidence angle, the material type, and the frequency are revealed, assuming both LC-RIS and conventional RISs are lossless. Then, the loss introduced by the LC-RIS is characterized, and the performance comparison in the lossy case is also given. In addition, the spatial radiation patterns of the LC-RIS and a conventional RIS are compared, and it is shown that the LC-RIS is an effective passive beamformer. Last, we provide a simulation on optimizing LC materials suitable for THz communications.

Switchable polymerizable Liquid Crystal Fresnel Zone Plates for Near Eye Displays

Zhiyu Xu, Camron Nourshargh, Alec Xu, Adithya Nair, Martin J. Booth, Steve J. Elston
and Stephen M. Morris

*Department of Engineering Science, University of Oxford, Parks Road, Oxford, OX1 3PJ,
United Kingdom*

In this study, we present a novel approach for the fabrication of Fresnel zone plates (FZPs) within polymerizable liquid crystal (LC) glass cells, employing Direct Laser Writing (DLW) technology. Fresnel zone plates, pivotal in the evolution of optical component design, focus light through diffraction—a method distinctly different from the refractive mechanism of conventional glass lenses. This principle enables the creation of lens structures that are markedly thinner, addressing the challenges associated with the bulk and weight of traditional lenses.

FZPs are categorized into three primary types: binary zone plates, staircase zone plates, and continuous zone plates. Each type demonstrates unique characteristics and fabrication complexities. Binary zone plates can be manufactured using traditional photolithography techniques with a photomask; however, the production of 3D staircase and continuous zone plates demands advanced precision 3D writing capabilities within LC system. This necessity underscores the importance of employing DLW technology, which offers unparalleled precision in the microfabrication of these intricate optical elements. The use of polymerizable LCs in constructing FZPs not only demonstrates the adaptability of these materials but also their potential in ushering a new era of miniaturized and efficient optical devices. Our methodology exemplifies the precision and flexibility of DLW in optical microfabrication, laying the groundwork for future advancements in the development of lightweight and compact optical systems.

3D Laser Sculpted Tunable Diffractive Optics Elements in Liquid Crystal Devices

Zimo Zhao, Bohan Chen, Patrick S. Salter, Martin J. Booth, Steve J. Elston, and Stephen M. Morris

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

Multi-element and multi-wavelength switchable diffractive optical elements will be demonstrated using two-photon polymerization direct laser writing in polymerizable nematic liquid crystal (LC) devices. Multielement two-dimensional Dammann gratings and computer-generated holograms will be presented that show that with an electric field the diffractive optic elements can be made to do one of a number of things such as turn on and off, tune to work at different wavelengths, and/or transform into other diffractive optic elements. All of these functionalities can be achieved with simple electrode configurations.

To begin with, single diffractive optical elements will be demonstrated in a LC layer by exploiting the 3D capabilities of the laser microfabrication technique. It will be shown that the behaviour of the device can be controlled by varying the voltage applied during fabrication process. The devices are shown to have a high diffraction efficiency of around 60% and fast response times compared with regions of the LC device that do not consist of the laser-written elements. Multi-element devices will then be presented that can generate a range of different patterns in the far-field, with each element being written at different depths within the LC layer. These different diffraction patterns can then be activated in the replay field with the application of different voltage amplitudes. These compact, transmissive, and switchable LC diffractive optical elements have excellent potential in applications including programmable beam shaping, microscopy, augmented reality/virtual reality displays, and optical communication systems.