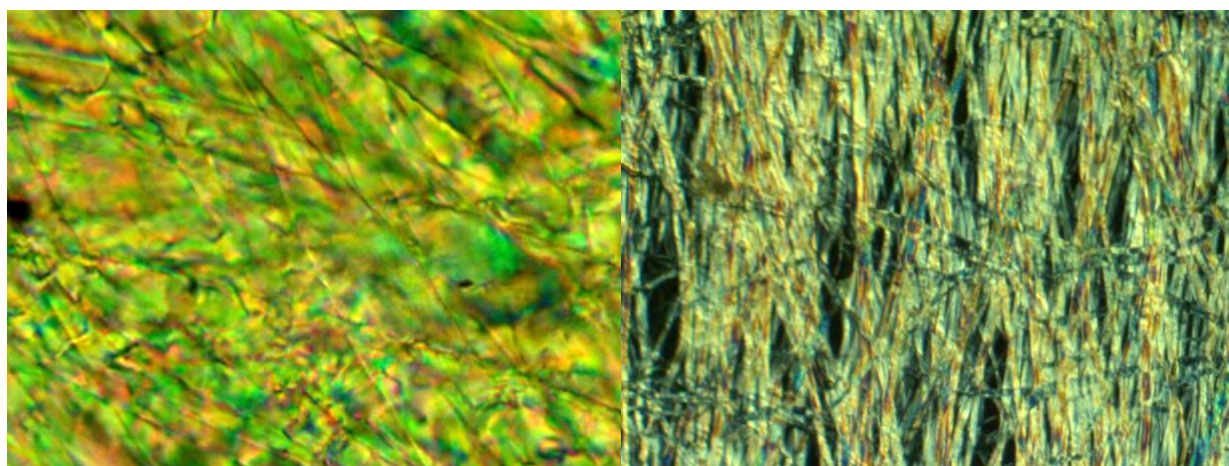


# Annual Conference of the British Liquid Crystal Society

11-13 April 2022

University of the West of England



Taylor & Francis Group  
an informa business

**IOP** Publishing

## Location:

Enterprise 1 Building  
University of the West of England (UWE)  
Frenchay Campus  
Coldharbour Lane  
Bristol  
BS16 1QY



## Parking

The parking space in front of EP1 can be accessed via the West Gate, past the MOD. Please press buzzer and tell security that you are attending the BLCS conference.

Dear all,

Thank you for joining the first in-person BLCS conference in two years.

It is your conference, and you need to work.

Use it to practice your conference skills. Ask stupid questions, network, entertain your audience, be captivating,

Taylor and Francis and IoP publishing generously sponsored the drinks. Without their contribution you would not be able to taste Uley beer. Maybe, I ordered too much, but I wanted to be on the safe side. Make sure that you not only drink the beer they paid but also visit their stalls. You will be their future authors.

Have fun and enjoy Bristol

Susanne and the team (the ones in the CFPR t-shirts)

# Programme

## Monday, the 11<sup>th</sup> of April 2022

11:00 to 12:30 Registration, tea and coffee

12:30 to 14:00 lunch

Chair: Claudio Zannoni

Time	Title	Name
14:00	Welcome	
14:15	Presentation by winner of the BLCS Young Scientist Prize	Joseph Cousins
14:45	Conformal maps for nematic colloids	Alexander J.H. Houston
15:05	Limits on characterising novel liquid crystals in optically thin cells	Denitsa Bankova

15:10 to 15:40 tea and coffee

Chair: Rebecca Walker

15:40	Hybrid-aligned films of smectic liquid crystals of polymers: coarse grained simulations	Emma Wood
16:00	Solution landscapes of the Ericksen-Leslie model and its comparison with the Landau-de Gennes model	Yucen Han
16:20	Multiscale modelling of bent liquid crystal Dimers	Gary Yu
16:40	Alignment layers for liquid crystals	Tom Moorhouse
17:00	Close of the day	

## Tuesday, the 12<sup>th</sup> of April 2022

Chair: Nigel Mottram

Time	Title	Name
10:00	Gray medal talk	Claudio Zannoni

11:00 to 11:30 tea and coffee

Chair: Mamatha Nagaraj

11:30	The effect of intrinsic chirality on modulated and polar nematic phases	Rebecca Walker
11:50	Light-responsive bent-core liquid crystals as candidates for energy harvesting	Ivan Dominguez-Candela
12:10	The influence of lateral substituents on the formation of the ferroelectric nematic phase	Ewan Cruickshank
12:30	AGM	

13:00 to 14:30 lunch

Chair: Helen Gleeson

14:30	Nematic liquid crystal rivulets	A.S. Bhadwal
14:50	Light-responsive lyotropic liquid crystal dispersions for controlled release	Beatrice E. Jones
15:10	Liquid crystalline order in nanostructures prepared through polymerization induced self-assembly (PISA)	Bartłomiej Czubak

15:30 to 16:00 tea and coffee

Chair: Alfonso Martinez-Felipe

16:00	Aggregation induced emission and liquid crystals	Jordan Hobbs
-------	--	--------------

16:20	Triphenoxazoles: A versatile material with applications as biological dyes and organic electronics	Owen M. Jones
16:50	The design of novel liquid crystal droplets as biosensors	Adele A Parry

17:00 to 19:00 Drinks (sponsored by Taylor and Francis and IoP publishing) and poster session

19:30 Conference dinner

## Wednesday, the 13<sup>th</sup> of April 2022

Chair: Joseph Cousins

Time	Title	Name
10:30	The investigation of dimeric nematogens linked to polysiloxane main chains	Wanhe Jiang
10:50	Synthesis and characterisation of a new liquid crystal dimers exhibiting the heliconical twist-bend smectic (SmCTB) phase	Calum J. Gibb

11:10 to 11:40 tea and coffee

Chair: Susanne Klein

11:45	Sturgeon lecture	Helen Gleeson
12:45	Close of conference	

13:00 to 14:00 lunch

# Oral Presentations



Joseph Cousins:

Surprise presentation by winner of  
the BLCS Young Scientist Prize

# Conformal Maps for Nematic Colloids

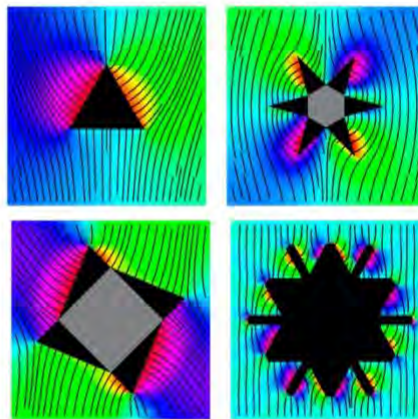
Alexander J.H. Houston<sup>1,\*</sup> and Gareth P. Alexander<sup>1,2</sup>

<sup>1</sup>*Department of Physics, Gibbet Hill Road, University of Warwick, Coventry, CV4 7AL, United Kingdom.*

<sup>2</sup>*Centre for Complexity Science, Zeeman Building,  
University of Warwick, Coventry, CV4 7AL, United Kingdom.*

Colloidal inclusions transform the behaviour of nematics, inducing topological defects and distortions that mediate anisotropic elastic interactions [1]. A multipole description of the far-field distortions underpins the theoretical modelling of these interactions and may also be used to characterise the response of active nematics [2]. It has been shown that colloidal geometry provides a route to determine the multipole structure with odd-sided regular polygons producing dipoles and even-sided ones quadrupoles [3]. Better understanding the connection between colloidal geometry and the structure of nematic distortions will open up routes for the design of novel soft metamaterials and the generation of propulsive and rotational modes in active nematics.

Determining the nematic director in the presence of a colloid with strong anchoring amounts to solving the Laplace equation subject to Dirichlet boundary conditions. This is difficult in non-trivial geometries but can be achieved by constructing conformal maps to simpler domains. By calculating the appropriate transformations we provide exact analytical solutions for a two-dimensional nematic in response to an arbitrary colloid. This allows the quantitative description of many observed phenomena but also reveals subtle orientation-dependency in the effects of concavity and chirality. In the latter case we show that this orientation dependence can be overcome by increasing the number of teeth on a chiral cog to produce persistent spontaneous rotation in an active nematic, allowing useful work to be extracted and serving as a first step in the development of micro-scale machines. The phase diagram for the chiral response as a function of cog shape was determined, along with principles for optimal design. We also use these methods to design colloids that extend the diversity of induced distortions beyond quadrupoles to arbitrary high multipoles, leading to strongly screened elastic distortions and highly angle-dependent interactions, with applications for novel metamaterials.



Exact analytic solutions for the director around a triangle, hexagonal star, chiral cog and a colloid producing a 14-pole distortion.

---

\* Electronic address: A.Houston@warwick.ac.uk

- [1] P. Poulin, H. Stark, T.C. Lubensky, and D.A. Weitz. Novel colloidal interactions in anisotropic fluids. *Science*, 275(5307):1770–1773, 1997.
- [2] A.J.H. Houston and G.P. Alexander. Defect loops in three-dimensional active nematics as active multipoles. *Phy. Rev. E*, in press (arXiv:2106.15424), 2022.
- [3] C.P. Lapointe, T.G. Mason, and I.I. Smalyukh. Shape-controlled colloidal interactions in nematic liquid crystals. *Science*, 326(5956):1083–1086, 2009.

# Limits on characterising novel liquid crystals and optically thin cells

Denitsa Bankova<sup>1\*</sup>, Nicolas Brouckaert<sup>1</sup>, Nina Podoliak<sup>1</sup>, Benjamin Beddoes<sup>1</sup>, Eleanor White<sup>1</sup>, Oleksandr Buchnev<sup>2</sup>, Malgosia Kaczmarek<sup>1</sup> and Giampaolo D'Alessandro<sup>3</sup>

<sup>1</sup> School of Physics and Astronomy, University of Southampton, Southampton, UK

<sup>2</sup> Optoelectronics Research Centre, University of Southampton, Southampton, UK

<sup>3</sup> School of Mathematical Sciences, University of Southampton, Southampton, UK

\* Author for Correspondence: [d.o.bankova@soton.ac.uk](mailto:d.o.bankova@soton.ac.uk)

New liquid crystal devices often require the use of optically thin cells and new liquid crystal materials. This leads to the following two challenges: (1) the total phase lag of the liquid crystal cells is smaller than  $2\pi$  (optically thin cells), and (2) the liquid crystal optical and dielectric properties are only partially known (novel materials). We explore the limit of the optical characterisation of thin liquid crystal cells and liquid crystals with incomplete set of data sheet parameters for Cross-Polarised Intensity (CPI) measurements in planar liquid crystal cells. The CPI method was successfully used before for optically thick cells to estimate several parameters, including the splay and bend elastic constants, viscosities, cell thickness, pretilt and polar anchoring energy [1-3]. Here we show that even cells with a phase lag of approximately  $\pi$ , such as E7 liquid crystal in a  $1.5\mu\text{m}$  cell, can be fully characterised. Furthermore, the fitting of CPI traces requires the values of the liquid crystal refractive indices and dielectric coefficients, however these may not be determined for new liquid crystals. We estimate the errors on the fitted parameters associated with the uncertainty of the dielectric constants and refractive indices. We demonstrate that even if these values, in particular the refractive indices, are approximated, the impact on the estimated values of the elastic constants and other liquid crystal parameters may not be significant. These results show that new liquid crystals without a full set of data sheet parameters can be successfully characterised using CPI measurements.

**Acknowledgements:** The authors would like to thank Tim Sluckin, Tetiana Orlova, Eleni Perivolari and Elena Ouskova.

## References:

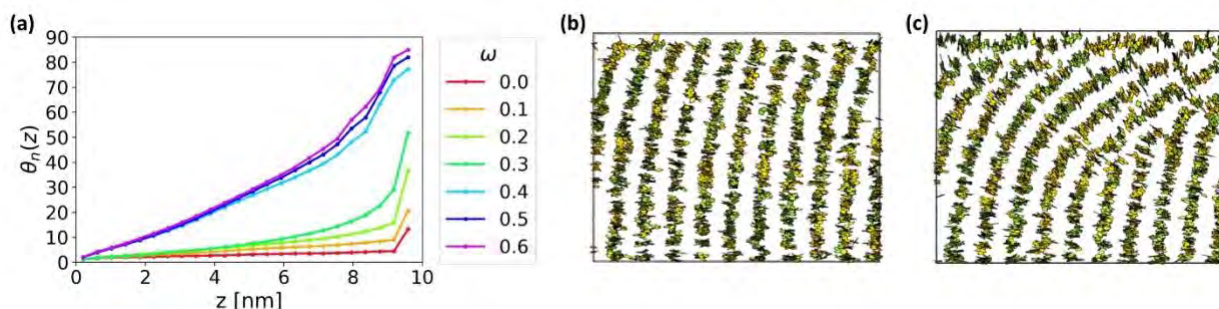
- [1] T. Bennett, et al., *Journal of Colloid and Interface Science*, **497**, 201 (2017).
- [2] T. Bennett, et al., *Applied Optics*, **56**, 9050 (2017).
- [3] E. Perivolari, et al., *Liquid Crystals*, **48**, 2086 (2021).

# Hybrid-Aligned Films of Sanidic Liquid Crystals of Polymers: Coarse-Grained Simulations

Emma L. Wood<sup>1</sup>, Anastasia Markina<sup>1</sup>, Kurt Kremer<sup>1</sup>, and Kostas Ch. Daoulas<sup>1</sup>

<sup>1</sup>Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany  
[\\*woode@mpip-mainz.mpg.de](mailto:*woode@mpip-mainz.mpg.de)

Soluble semiconducting polymers, comprising conjugated backbones and flexible side chains, are interesting for fabricating film-like active layers of electronic devices. These polymers form semi-crystalline or sanidic liquid crystalline (LC) lamellae, where layers of cofacially stacked backbones alternate with layers of side chains.<sup>1</sup> Uniformly-ordered lamellae, where the  $\pi$ - $\pi$  stacking direction of the polymers is orthogonal to the surfaces of the film, allow efficient vertical charge transport. Such “face-on” order is favoured at graphene surfaces, which are used as electrodes for photovoltaic cells. However, free surfaces at the top of films promote “edge-on” orientations, where the stacking direction is parallel to the surface.<sup>2</sup> Therefore, it is useful to study the deformation of sanidic LC lamellae in thin films with contrasting boundary conditions.



**Figure 1.** (a) Profiles  $\theta_n(z)$  for orientation of the stacking direction in films of P3HT as a function of  $z$  and  $\omega$ . (b, c) Visualisations of deformations in films with  $\omega = 0.2$  and  $\omega = 0.5$ , respectively.

Here, we focus on poly(3-hexylthiophene) (P3HT), and use a highly coarse-grained hindered-rotation model<sup>3,4</sup> to allow Monte Carlo simulations of lamellae in films with experimentally-relevant<sup>2</sup> thicknesses. Although each interaction site represents an entire monomer including its side-chain, the model describes lamellar order thanks to anisotropic nonbonded potentials.<sup>3,4</sup> Studying deformations requires a realistic potential for the relative orientations of the monomers, so we parameterise using density functional theory (DFT) calculations.

We investigate the textures of films with a strong preference for face-on order at the bottom surface, and various strengths  $\omega \geq 0$  for edge-on interactions at the top surface. We find that deformations are always present, and characterise them using profiles  $\theta_n(z)$  for the orientation of the stacking direction as a function of height  $z$  (Fig. 1a). When surface interactions are weak ( $0 \leq \omega \leq 0.3$ ), deformations are smooth (Fig. 1b). Increasing the strength ( $\omega = 0.3 \rightarrow 0.4$ ) causes a jump to a regime of stronger deformations which induce broken lamella defects (Fig. 1c). For constant  $\omega$ , changing the film thickness causes only a slight change in orientation at the top surface. Therefore, deformations in thicker films tend to be weaker, but defects appear at the same  $\omega$  for all studied film thicknesses. We correlate our observations to elastic properties of real materials via a simple phenomenological model.<sup>5</sup>

## References

- [1] D. M. DeLongchamp, R. J. Kline, E. K. Lin, D. A. Fischer, L. J. Richter, L. A. Lucas, M. Heeney, I. McCulloch and J. E. Northrup, *Advanced Materials*, 2007, 19, 833-837.
- [2] O. Dolynchuk, P. Schmode, M. Fischer, M. Thelakkat and T. Thurn-Albrecht, *Macromolecules*, 2021, 54, 5429-5439.
- [3] C. Greco, A. Melnyk, K. Kremer, D. Andrienko and K. Ch. Daoulas, *Macromolecules*, 2019, 52, 968-981.
- [4] E. L. Wood, C. Greco, D. A. Ivanov, K. Kremer and K. Ch. Daoulas, *J. Phys. Chem. B*, 2022, In Press.
- [5] M. Kleman and O. D. Lavrentovich, *Soft Matter Physics: An Introduction*, Springer, 2003.

# Solution Landscapes of the Ericksen-Leslie Model and its Comparison with the Landau-de Gennes Model

Yucen Han<sup>1\*</sup>; Jianyuan Yin<sup>2</sup>, Yucheng Hu<sup>3</sup>, Apala Majumdar<sup>1</sup>, and Lei Zhang<sup>4</sup>

<sup>1</sup> Department of Mathematics and Statistics, University of Strathclyde, Glasgow, G1 1XH, UK.

<sup>2</sup> Department of Mathematics, National University of Singapore, Singapore 119076.

<sup>3</sup> Beijing Advanced Innovation Center for Imaging Theory and Technology, Academy for Multidisciplinary Studies, Capital Normal University, Beijing 100048, People's Republic of China.

<sup>4</sup> Beijing International Center for Mathematical Research, Center for Quantitative Biology, Peking University, Beijing 100871, China.

There are different continuum mathematical theories for nematic liquid crystals (NLCs) such as the Ericksen–Leslie (EL) theory [1] and the celebrated Landau–de Gennes (LdG) theory [2]. Each theory corresponds to a macroscopic order parameter that is a measure of the degree of orientational order or state of NLC anisotropy. The solution landscape is a collective term used to describe the plethora of admissible stable or unstable configurations and relationships between them, in a given setting. To compare models, we investigate the solution landscapes of the EL vector model and LdG Q-tensor model for NLCs, confined in a two-dimensional square domain with tangent boundary conditions. There are many similarities, including the stable states, bifurcation behaviours and sub-solution landscapes with low-index saddle solutions in Fig 1. Significant disparities also exist between the two models. The EL model exhibits new stable solutions with interior defects, high-index ‘fake defect’ solutions, novel tessellating solutions and certain types of distinctive dynamical pathways.

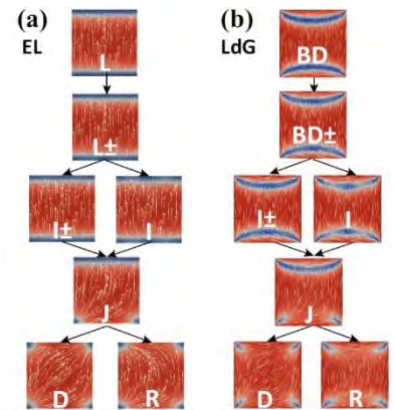


Fig 1: Sub-solution landscapes for (a) EL and (b) LdG models

The comparison between multiple models, either theoretically or numerically, is interesting but challenging. Our solution landscape approach that delves into the connectivity of unstable and stable states provides a comprehensive and efficient way for model comparison. This approach is applicable to a wide range of mathematical models in physics beyond liquid crystal theory.

**Acknowledgements:** Y.Han acknowledges support from a Royal Society Newton International Fellowship. LZ was supported by the National Natural Science Foundation of China. LZ and AM acknowledge support from a Royal Society Newton Advanced Fellowship. AM acknowledges support from the University of Strathclyde New Professor's Fund, a Leverhulme International Academic Fellowship, an OCIAM Visiting Fellowship at the University of Oxford, a visiting professorship at the University of Bath and IIT Bombay. JY acknowledges support from the Elite Program of Computational and Applied Mathematics for PhD Candidates of Peking University.

## References:

- [1] de Gennes PG, Prost J. The physics of liquid crystals, vol. **83**. Oxford, UK: *Oxford University Press* (1993).  
 [2] Ericksen JL. Liquid crystals with variable degree of orientation. *Arch. Ration. Mech. Anal.* **113**, 97–120 (1991).

\* Author for Correspondence: [yucen.han@strath.ac.uk](mailto:yucen.han@strath.ac.uk)

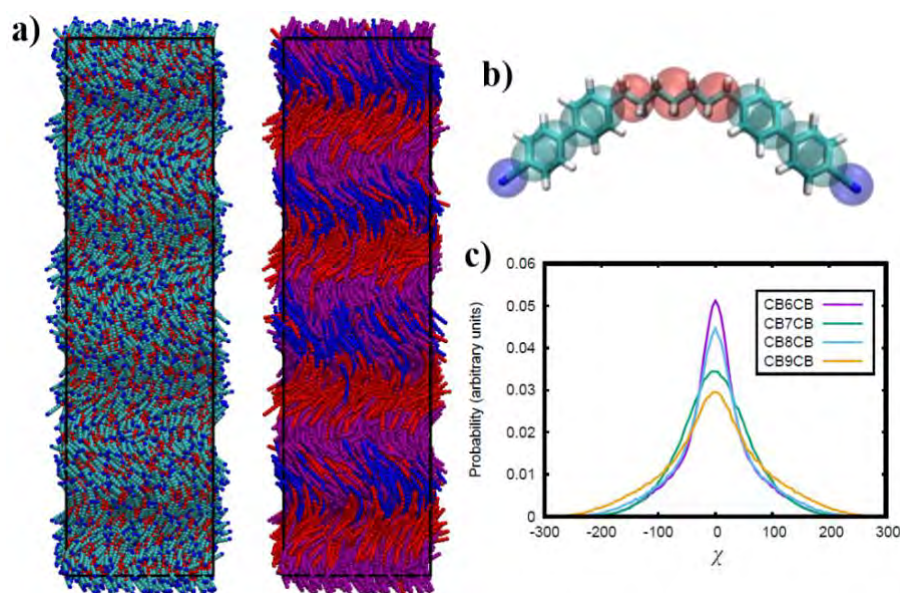
# Multiscale Modelling of Bent Liquid Crystal Dimers

Gary Yu<sup>1</sup> and Mark R. Wilson<sup>1</sup>

<sup>1</sup>Department of Chemistry, Durham University, Durham, DH1 3LE, UK

\*gary.yu@durham.ac.uk

The bent liquid crystal dimer CB7CB, is known to exhibit the twist-bend nematic ( $N_{TB}$ ) phase, which features a heliconical structure despite the achiral nature of the mesogen [1]. We present extensive all-atom molecular dynamics simulations of CB7CB. The simulated  $N_{TB}$  phase has structural characteristics in good agreement with experiment and, upon heating, shows the full phase diagram with transitions into the N and I phases. Distributions for the bend angle and chirality order parameter [2],  $\chi$ , calculated for a wide range of dimers provide a measure of the conformational distributions, and the effect of the spacer length or heteroatom linkages to be explored. It is demonstrated that these mesogens are statistically achiral but can adopt conformers with high helical twisting powers which have no preference for a specific handedness. Single-molecule stochastic dynamics simulations in the gas phase, coupled with the various analyses, are shown to be a viable route to high-throughput analysis of similar systems. Using the multiscale coarse-graining method, a coarse-grained model (where multiple atoms are grouped into single interaction sites) was parametrised using an all-atom reference of the  $N_{TB}$  phase. The resulting model exhibits the  $N_{TB}$  phase, with good accuracy, and provides a 12x speed up compared to a full atomistic representation. Upon heating, the coarse-grained system successfully captures the  $N_{TB}$ -N and N-I phase transitions and the spontaneous growth of the N and, subsequent,  $N_{TB}$  phases from cooling of the I phase. This demonstrates a novel and simple application of an automated procedure to develop highly representative and transferable coarse-grained models for thermotropic liquid crystals.



**Figure 2: (a) Simulation snapshots from coarse-grained modelling of the  $N_{TB}$  phase. (b) Molecular structure of CB7CB with its coarse-grained mapping scheme. (c) Chirality order parameter,  $\chi$ , distributions for  $CB_nCB$ .**

## References

- [1] M. Cestari, et al., *Phys. Rev. E*, 2011, 84, 031704
- [2] B.-C. Kim, et al., *RSC Adv.*, 2018, 8, 1292

# Novel Methods for Fabricating Metasurface Alignment Layers for Liquid Crystal Devices

Moorhouse, Tom<sup>1</sup>; Jones, J. Cliff<sup>1\*</sup>

<sup>1</sup> Department of Physics, University of Leeds, Leeds, UK

Surface alignment of the liquid crystal (LC) director can be controlled in a variety of ways; some relying on polymer orientation at a polymer-LC interface, such as mechanical rubbing or photoalignment, and others that rely on topographic surface patterning, as is the case with grating aligned LCs. Surface relief structures, such as linear gratings, have not only shown the ability to uniformly align the LC director [1], but also induce sufficient elastic distortion of the director field, giving rise to bistable surface alignments; as demonstrated in the Zenithal Bistable Display (ZBD) [2]. For display applications, grating structures often need to be index matched to the surrounding LC to avoid unwanted optical diffraction. Alternatively, a sub-optical grating pitch has the potential to suppress first order diffraction modes, without the need for index matching, whilst retaining uniform LC director alignment [3].

In this work, surface relief structures are patterned in to a shape memory polymer (SMP) and subsequently miniaturized, reducing the pitch and increasing the depth of the original structure [4]. Nano-imprint lithography (NIL) is used to create dry-etch masks upon the SMP, to facilitate anisotropic dry etching for pattern transfer in to the SMP surface [5]. Once characterized, the resulting structures are replicated and embossed into LC alignment polymers to explore their effects on alignment uniformity and anchoring strength within the LC medium, primarily studied using Polarizing Optical Microscopy (POM). Focus is placed on achieving sub-micron and sub-optical surface geometries, using a miniaturization technique that strives to avoid the experimental limitations and complexities of sub-micron photolithography [6].

**Acknowledgements:** This work was funded by the EPSRC. JCJ wishes to thank the EPSRC for a Fellowship in Manufacturing (EP/L015188/1).

## References:

- [1] D. W. Berreman, *Phys. Rev. Lett.*, **28**, 26, 1683–1686 (1972)
- [2] J. C. Jones, *Liquid Crystals*, **44**:12-13, 2133-2160 (2017)
- [3] D. C. Flanders et al., *Appl. Phys. Lett.* **32**(10), 597-598 (1978)
- [4] X.-M. Zhao et al., *Sensors and Actuators A* **65** (1998)
- [5] S. Sayed, P.R. Selvaganapathy, *Nanoscale Advances*, **2**, 5461 (2020)
- [6] C.-Y. Wu et al., *Micromachines*, **10**, 547 (2019)

\* Author for Correspondence: [j.c.jones@leeds.ac.uk](mailto:j.c.jones@leeds.ac.uk)

Claudio Zannoni:

Surprise presentation by the winner of the Gray medal



# The Effect of Intrinsic Chirality on Modulated and Polar Nematic Phases

Walker, Rebecca<sup>1\*</sup>; Pociecha, Damian<sup>2</sup>; Cruickshank, E.<sup>1</sup>; Storey, John MD<sup>1</sup>; Gorecka, Ewa<sup>2</sup> and Imrie, Corrie T<sup>1</sup>

<sup>1</sup> Department of Chemistry, University of Aberdeen, Aberdeen, United Kingdom

<sup>2</sup> Department of Chemistry, University of Warsaw, Warsaw, Poland

Liquid crystals are ideal systems to study chirality, its origins and chirality propagation, and enhancing our fundamental knowledge of these phenomena may hold the key to an understanding of the origins of life. The twist-bend nematic phase,  $N_{TB}$ , is an intriguing and unique example of spontaneous mirror symmetry breaking in a fluidic state; a locally chiral phase formed from achiral molecules. Directors in the  $N_{TB}$  phase map out a heliconical structure, the formation of which is not related to molecular chirality.[1] Here we demonstrate how the  $N_{TB}$  phase having spontaneous structural chirality responds at a microscopic level to the presence of intrinsic molecular chirality, and discuss new examples of the rarely observed chiral twist-bend nematic phase,  $N^*_{TB}$  in both covalently- and hydrogen-bonded mesogens.[2]

A second intriguing variant of the nematic phase is the polar, achiral ferroelectric nematic phase,  $N_F$ , experimentally discovered in 2017 and thus far only observed in a handful of molecules.[3] The combination of ferroelectricity with nematic-like fluidity and ease of processing has enormous potential for applications. Until very recently, the combination of chirality and polar order in soft matter had been observed only in smectic [4] and columnar phases [5]. The only reports to date of chiral  $N_F^*$  phases have been for achiral nematogens doped with chiral additives [6]; here we describe the first examples of intrinsically chiral ferronematogens, and the influence of this inherent molecular chirality on the structure of this new polar phase.

## References:

- [1] V. Borshch *et al.*, *Nat. Commun.*, **2013**, *4*, 2635
- [2] R. Walker, *et al.*, *Chem. - A Eur. J.* **2019**, *25*, 13329–13335; R. Walker, *et al.*, *Mater. Adv.* **2020**, *1*, 1622–1630.
- [3] R. J. Mandle, *et al.*, *Chem. – A Eur J.*, **2017**, *23*, 14554-14562; J. X. Li, *et al.*, *Science Advances*, **2021**, *7*.
- [4] C. Loubser, *et al.*, *J. Mater. Chem.*, **1994**, *4*, 71-79.
- [5] H. Takezoe, *et al.*, *Rev. Mod. Phys.* **2010**, *82*, 897.
- [6] H. Nishikawa *et al.* *Adv. Mater.* **2021**, *33*, 2101305; X.H. Zhao, *et al.*, *Proc. Natl. Acad. Sci. U.S.A.* **2021**, *118*, e2111101118; C. Feng *et al.*, *Adv. Optical Mater.* **2021**, *9*, 2101230.

\* Author for Correspondence: [rebecca.walker@abdn.ac.uk](mailto:rebecca.walker@abdn.ac.uk)

## Light-responsive bent-core liquid crystals as candidates for energy harvesting

Ivan Dominguez-Candela<sup>1,3</sup>, Iman Zulkhairi<sup>1</sup>, Inmaculada Pintre<sup>4</sup>, Jaime Lora-Garcia<sup>2</sup>, Vicent Fombuena<sup>3</sup>, Blanca Ros<sup>4</sup>, Alfonso Martinez-Felipe<sup>1,5</sup>

<sup>1</sup>Chemical Process and Materials Research Group, School of Engineering, University of Aberdeen, King's College, Aberdeen AB24 3UE, Scotland, UK.

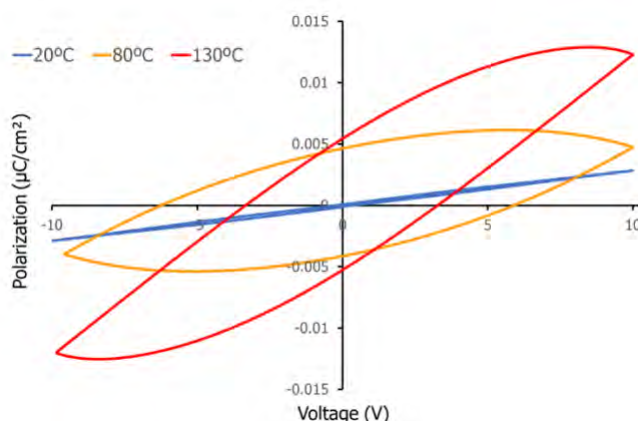
<sup>2</sup>Instituto de Seguridad Industrial, Radiofísica y Medioambiental (ISIRYM) Universitat Politècnica de València (UPV), Plaza Ferrándiz y Carbonell, s/n 03801 Alcoy, Spain.

<sup>3</sup>Technological Institute of Materials (ITM), Universitat Politècnica de València (UPV), Plaza Ferrándiz y Carbonell 1, 03801 Alcoy, Spain.

<sup>4</sup>Instituto de Nanociencia y Materiales de Aragón, Departamento de Química Orgánica, Facultad de Ciencias, Universidad de Zaragoza-CSIC, Campus San Francisco, E-50009 Zaragoza, Spain.

<sup>5</sup>Centre for Energy Transition, University of Aberdeen, King's College, Aberdeen AB24 3UE, Scotland, UK.

The development of innovative materials that can improve the efficiency of renewable energy technologies will play a decisive role to reduce greenhouse emissions and reach net-zero targets globally<sup>[1]</sup>. Liquid crystals are exciting candidates as advanced materials for green technologies, due to their ability to interact with, and respond to, external sources, resulting in tailor-made nanostructures<sup>[2]</sup>. More specifically, azobenzene-containing compounds can exhibit liquid crystalline phases controllable by light excitation, *via trans-to-cis* photoisomerisation, providing mechanisms for energy conversion from solar sources<sup>[3]</sup>. If these phenomena are coupled to ferroelectric response, we can unveil new pathways to promote photo-electric energy conversion and storage. In this work, we show some results obtained on light-responsive ferroelectric liquid crystals. Among others, we have studied mixtures of bent-core molecules (showing anticlinic smectic C antiferroelectric polar phases) with small concentrations of azobenzene groups. We have assessed their dielectric and ferroelectric response, as a function of temperature and phase behaviour. In addition, we have evaluated the effect of UV-light illumination on electric polarization and conductivity, to assess their potential as light harvesters. We believe that our work can open new frontiers for liquid crystals in photovoltaic and sensing applications.



Hysteresis loops obtained at different temperatures for a mixture of bent-core liquid crystals, containing 5% (molar %) of azobenzene molecules.

### References

1. International Energy, A., *Global Energy Review 2020*. 2020, IEA: Paris.
2. Shen, Y. and I. Dierking, *Perspectives in Liquid-Crystal-Aided Nanotechnology and Nanoscience*. Applied Sciences-Basel, 2019. **9**(12): p. 2512-2512.
3. Gong, M., et al., *Optimizing energy harvesting performance of silicone elastomers by molecular grafting of azobenzene to the macromolecular network*. Rsc Advances, 2021. **11**(31): p. 19088-19094.

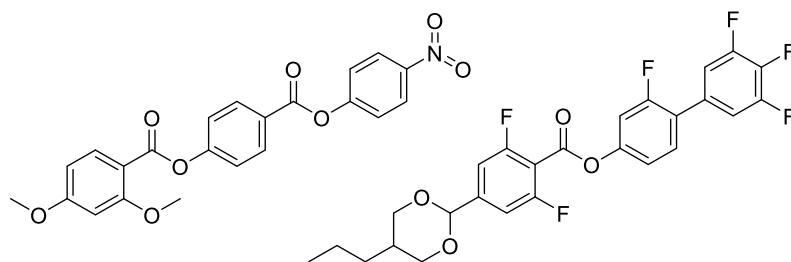
# The Influence of Lateral Substituents on the Formation of the Ferroelectric Nematic Phase

Cruickshank, Ewan<sup>1\*</sup>; Brown, Stevie<sup>1</sup>; Walker, Rebecca<sup>1</sup>; Majewska, Magdalena<sup>2</sup>; Makal, Anna<sup>2</sup>; Pocięcha, Damian<sup>2</sup>; Górecka, Ewa<sup>2</sup>; Storey, John<sup>1</sup> and Imrie, Corrie<sup>1</sup>

<sup>1</sup>Department of Chemistry, School of Natural and Computing Sciences, University of Aberdeen, Aberdeen, AB24 3UE, UK

<sup>2</sup>University of Warsaw, Faculty of Chemistry, ul. Żwirki i Wigury 101, 02-089, Warsaw, Poland

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, two groups independently reported the discovery of a new type of nematic phase in two different compounds named: RM734 [1] and DIO [2], **Figure 1**. This phase is ferroelectric in nature and thus termed the ferroelectric nematic phase, N<sub>F</sub> [3]. While RM734 and DIO, in terms of their chemical structures, appear to be rather different to each other, they do both share a large longitudinal dipole moment. The polar ordering within the N<sub>F</sub> phase allows for the phase to be much more sensitive to electric fields than the nematic phase and so the phase could be transformative in electro-optic technologies. There are still only a limited number of materials which have been shown to exhibit the N<sub>F</sub> phase [4-7] and it is crucial that the library of compounds showing it is expanded in order to gain a greater understanding of the properties driving its formation. Here we report the transitional properties of a series of three ring materials containing lateral substituents which display the desired ferroelectric nematic phase.



**Figure 1.** Molecular structures of RM734 (left) and DIO (right).

- [1] Mandle, R. J. et al. *Phys. Chem. Chem. Phys.* **19**, 11429–11435 (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. et al. *Chemistry-a European Journal*, **23**, 14554-14562 (2017).
- [5] Li, J. et al. *Science Advances*, **7**, eabf5047, (2020).
- [6] Manabe, A. et al. *Liq. Cryst.* **48**, 1079-1086, (2021).
- [7] Brown, S. et al. *ChemPhysChem*, **22**, 2506-2510, (2021).

**Acknowledgements:** This work was financially supported by the Engineering and Physical Sciences Research Council [EP/V048775/1].

\*Author for Correspondence: [s02ec1@abdn.ac.uk](mailto:s02ec1@abdn.ac.uk)

# Nematic liquid crystals rivulets

A.S. Bhadwal<sup>1\*</sup>; J.R.L. Cousins<sup>2,3</sup>; N.J. Mottram<sup>2</sup>; S.K. Wilson<sup>3</sup>; I.C. Sage<sup>1</sup>; and C.V. Brown<sup>1</sup>

<sup>1</sup>School of Science and Technology, Nottingham Trent University, Nottingham, UK

<sup>2</sup>School of Mathematics and Statistics, University of Glasgow, Glasgow, UK

<sup>3</sup>Dept. of Mathematics and Statistics, University of Strathclyde, Glasgow, UK

Free surface flow involves a mobile interface at the fluid-air boundary. A rivulet can be formed by a thread of fluid flowing down an inclined solid substrate, with the most familiar example of rivulets being drops of rainwater flowing down a windowpane. Rivulets also occur in a wide variety of physical contexts and over-length scales spanning from nano to geophysical levels [1, 2]. A substantial amount of experimental and theoretical work exploring the free surface flow of isotropic rivulets has been reported in the literature [3, 4]. However, there is a paucity of work on the free surface flow of non-Newtonian and anisotropic micro- to millimeter scale rivulets.

Anisotropic nematic liquid crystals are particularly interesting for these studies since they offer unique controllability of internal ordering and orientation of the nematic director, and hence localized control of the effective viscosity. This provides a unique route to also dynamically manipulate the localized free surface shapes that can be adopted by a flowing nematic liquid and provides an insight into the competition between nematic flow alignment, surface alignment, and electric field alignment forces.

We have observed the influence of electric fields on the free surface of a straight nematic rivulet that has pinned contact lines. The rivulet flow was constrained along a homeotropic wetting patch by chemically patterning the solid substrate. In the absence of the electric field the liquid crystals director flow aligns at the Leslie angle, with no change in the free surface shape of the rivulet. On the application of localized A.C. voltage orthogonal to the direction of the rivulet flow, electrically induced nematic director re-orientation results in a change in the effective bulk viscosity of the nematic liquid crystal material. In the electric field region, the flow rate locally decreases, the height of the rivulet increases, and the cross-sectional shape of the rivulet and the contact angles also change. These observations are found to be consistent with the results of theoretical model based on Ericksen-Leslie equations.

**Acknowledgments:** This work was funded by EPSRC research grants (EP/T012986/1 and EP/T012501/2).

## References:

- [1] A.A. Darhuber and S.M. Troian, *Annu. Rev. Fluid Mech.*, **37**, 425 (2005).
- [2] R.W. Griffiths, *Annu. Rev. Fluid Mech.*, **32**, 477 (2000).
- [3] G.D. Towell, and L.B. Rothfeld, *AIChE Journal*, **12**, 972 (1966).
- [4] C. Paterson, et al., *Eur. J. Mech. B Fluids*, **41**,94 (2013).

\* Author for Correspondence: [akhshay.bhadwal@ntu.ac.uk](mailto:akhshay.bhadwal@ntu.ac.uk)

## Light-Responsive Lyotropic Liquid Crystal Dispersions for Controlled Release

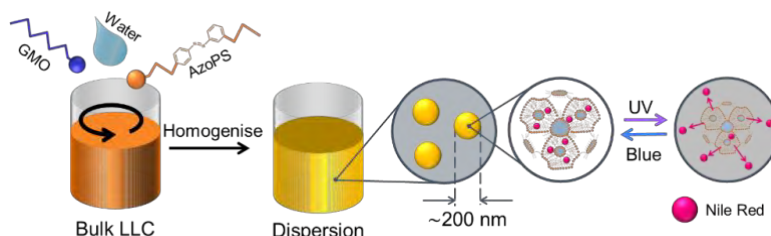
Beatrice E. Jones,<sup>1,2</sup> Elaine A. Kelly,<sup>1</sup> Nathan Cowieson,<sup>2</sup> Giorgio Divitini<sup>1</sup> and Rachel C. Evans<sup>1</sup>

<sup>1</sup> Department of Materials Science and Metallurgy, University of Cambridge, <sup>2</sup> Diamond Light Source, Oxfordshire, UK

[bej28@cam.ac.uk](mailto:bej28@cam.ac.uk)

Creating stimuli-responsive materials is crucial to advance controlled delivery systems for drugs and catalysts. Lyotropic liquid crystals (LLCs), formed from the self-assembly of amphiphiles on the addition of a solvent, have complex, nanoscale internal structures that can entrap guest molecules by restricting diffusion out of these networks.<sup>1</sup> These LLCs can be broken up in excess aqueous solution using a high-shear input to form dispersions of nanoparticles. This aids their application as delivery systems, whilst retaining an ordered LLC interior required for entrapment.<sup>2</sup> Previous studies have incorporated photoswitchable functional groups into amphiphiles to create LLCs whose structure can be modified using light as an external stimulus.<sup>3,4</sup> This work aims to combine the effects of light-responsive LLCs into nanodispersions that are suitable as delivery systems, enabling control over the LLC structure and subsequent release of guest molecules using light.

Here, two different light-responsive azobenzene photosurfactants (AzoPS) contain a neutral tetraethylene glycol head group, alkyl spacer (of chain length 4 or 8), azobenzene moiety and alkyl tail (of length 6 or 8). When combined into glycerol monooleate–water systems (10–30 wt%), these form either ordered hexagonal or lamellar LLC phases, depending on the chain length of the AzoPS. Homogenisation forms stable dispersions of particles ~200 nm in diameter with internal bicontinuous diamond cubic phases, as seen by small-angle X-ray scattering and cryo-transmission electron microscopy. On irradiation with UV light, rapid isomerisation of the azobenzene from the *trans* to *cis*-predominant states occurs within seconds. The bicontinuous diamond cubic structure remains after isomerisation, but the lattice parameter decreases by up to 39%. This is due to “bending” of the AzoPS tail in the *cis* state, changing the tail volume and contracting the cubic lattice. Dye-loading experiments show that this lattice contraction results in release of Nile Red from the LLC matrix, confirmed by a 72% decrease in the fluorescence intensity as it moves from the lipid-like LLC matrix into the aqueous phase. This rapid release occurs within minutes, contrasting the minimal diffusion from the matrix measured over 3 hours. The ability to use light to tune the internal structure of these LLC dispersions, leading to dramatic effects on their ability to retain small molecules, suggests these systems have huge potential for controlled delivery and release applications.



**Figure 1.** Schematic diagram showing the formation of light-responsive LLC dispersions. Isomerisation of the AzoPS using UV light results in a decrease in cubic lattice parameter and release of the dye, Nile Red.

### References:

1. Mulet, X.; Boyd, B.; Drummond, C. *J. Colloid Interface Sci.*, 2013, **393**, 1.
2. Amar-Yuli, I.; Wachtel, E. *et al.*, *Langmuir*, 2007, **23**, 3637.
3. Peng, S.; Guo, Q. *et al.*, *J. Mater. Chem. C*, 2014, **2**, 8303.
4. Houston, J.; Kelly, E. A. *et al.* *J. Mater. Chem. C*, 2019, **7**, 10945

# Liquid crystalline order in nanostructures prepared through polymerization induced self-assembly (PISA)

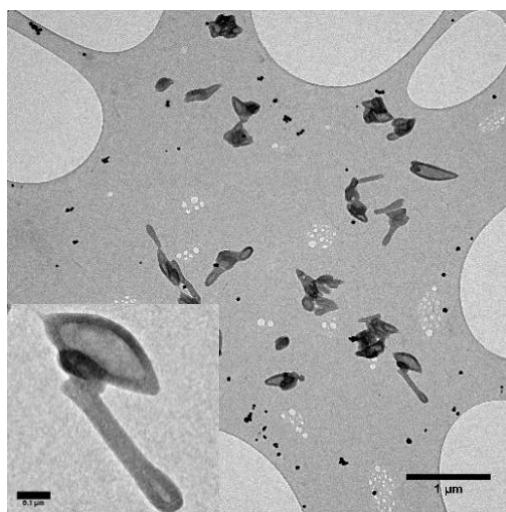
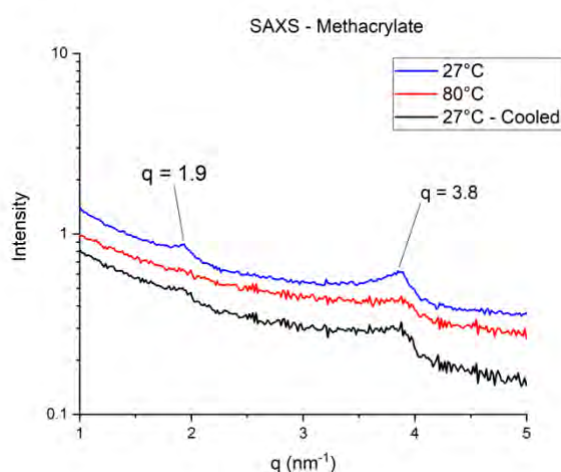
Czubak, Bartłomiej<sup>1\*</sup>; Warren, J. Nicholas<sup>2</sup>; Nagaraj, Mamatha<sup>1</sup>

<sup>1</sup> School of Physics and Astronomy, University of Leeds, Leeds, United Kingdom

<sup>2</sup>School of Chemical and Process Engineering, University of Leeds, Leeds, United Kingdom

Polymerization induced self-assembly (PISA) is an efficient way of preparing monodisperse nano-objects from block copolymers through living radical polymerizations such as reversible addition-fragmentation chain transfer (RAFT) polymerization. Recently, perfluorinated monomers which possess liquid crystal (LC) groups have been used to expand the list of suitable PISA monomers.<sup>[1]</sup> Incorporation of such LC groups can introduce features such as thermal responsiveness and optical properties that are not usually associated with PISA nano-objects.<sup>[2]</sup> However, the influence of these two forms of self-assembly on each other in PISA remains unexplored.

In this presentation, we explore the influence of introducing LC groups on both the self-assembly processes, and on the subsequent characteristics observed in the synthesized nanomaterials. A detailed investigation of the self-assembled structures characterized using SAXS (Figure 1), WAXS, polarized light microscopy and electron microscopy (Figure 2) is performed. LC order in the particles is identified. The formation of the nanoobjects with focus on the LC order influence on the shape of the particles is described.



*Figure 1* – Small angle X-ray scattering (SAXS) patterns obtained for nanoobjects formed from methacrylic block copolymer with fluorinated liquid crystalline side groups. *Figure 2* – Transmission electron microscopy (TEM) image obtained for a single PISA prepared nanoobject.

## References:

- [1] M. Huo, D. Li, G. Song, J. Zhang, D. Wu, Y. Wei and J. Yuan, *Macromol. Rapid Commun.* 2018, 39, 1700840
- [2] L. Shen, H. Guo, J. Zheng, X. Wang, Y. Yang and Z. An, *ACS Macro Lett.* 2018, 7, 3, 287-292

\* Author for Correspondence: [pybcz@leeds.ac.uk](mailto:pybcz@leeds.ac.uk)

## Aggregation induced Emission and Liquid Crystals

[J. Hobbs](#)<sup>1\*</sup>, [J. Mattsson](#)<sup>1</sup>, [M. Nagaraj](#)<sup>1</sup>

<sup>1</sup>*School of Physics and Astronomy, University of Leeds, Leeds, United Kingdom*

*\*py14jh@leeds.ac.uk*

The fluorescence of liquid crystals (LCs) is often overlooked due to the low fluorescence intensity of many LCs. Understanding the photophysical properties of LCs, and those of fluorescent dopants added to LCs, could both significantly advance our fundamental understanding of LCs, and provide new directions for LC-based applications. Liquid crystals have been combined with fluorescent materials such as quantum dots [1,2], metal based nanoparticles [2] as well as other organic molecules [3]. However all these materials suffer from aggregation caused quenching of their fluorescence.

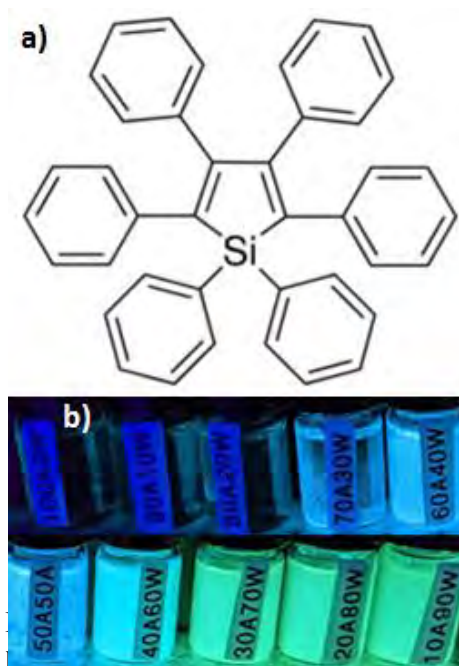
Aggregation-induced emission (AIE) is a phenomenon in which a material's fluorescence properties change with molecular aggregation. [4]. Figure 1a shows the chemical structure of an AIE active molecule, hexaphenyl silole (HPS). In its aggregated state the dissipation of energy through rotations of the external phenyl rings of the HPS molecule are restricted. Instead, HPS dissipates the excitation energy through fluorescence [4]. This results a material that is non-emissive in their isolated state and fluorescent in the aggregated state such as in figure 1b. The AIE effect can be activated and controlled by a number of parameters, including changes in the molecular environment [5].

AIE active materials have been suggested for a wide variety of applications from biological probes to chemical sensing and stimuli responses [4]. Combining the properties of AIEs with those of LCs has produced materials which show electro-luminescent properties as well as polarized luminescence both linear and circularly polarized [4] and while much work has been published on the synthesis of molecules that are both AIE active and liquid crystalline [4], little work outside of synthesis and the initial characterization of these materials has been conducted.

This presentation will provide a detailed study of the fluorescence behavior LCs when combined with AIE active molecules. The effects on the liquid crystallinity on the fluorescence and aggregation behavior of HPS will be presented, as determined using optical and fluorescence microscopy, fluorescence spectroscopy techniques.

### References

- [1] J. Mirzaei, et. al., *J. Mater. Chem.*, **22**, (2012).
- [2] U. Shivakumar, et. al., *Liquid Crystals*, **38**, 11-12, (2011).
- [3] Nowicka, K et. al., *Phase Transitions*, **87**, 10-11, (2014)
- [4] J. Mei, et. al., *Chem. Rev.*, **115**, 21, (2015)
- [5] J, Chen, et. al., *Chem. Mater.* **15**, 7, (2003)



**HPS in acetone and water.**

# Triphenoxazoles: A Versatile Material with Applications as Biological Dyes and Organic Electronics

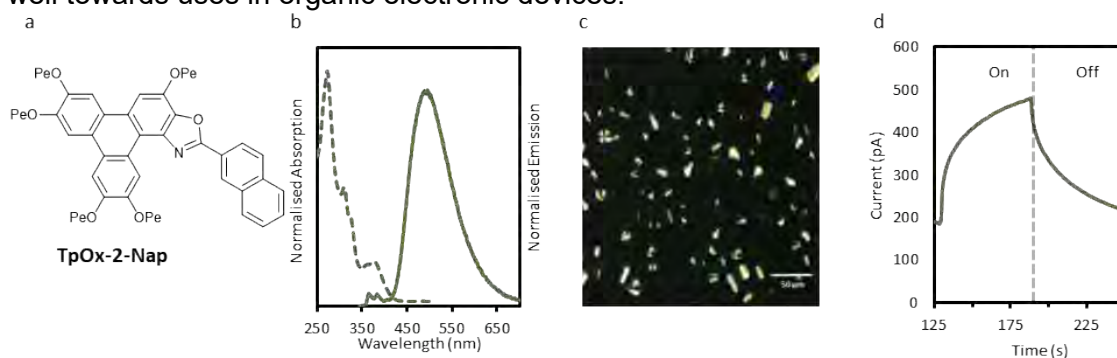
Owen M. Jones,<sup>a</sup> Gregory C. O'Callaghan,<sup>a</sup> Karolis Virzbickas,<sup>b</sup> Michael S. Butlin,<sup>a</sup> Dennis Zhao,<sup>a</sup> Alexander P. G. Robinson,<sup>b</sup> Jon A. Preece<sup>a</sup>

<sup>a</sup>School of Chemistry, University of Birmingham, UK, B15 2TT

<sup>b</sup>School of Chemical Engineering, University of Birmingham, UK, B15 2TT

E-mail: [o.jones.1@bham.ac.uk](mailto:o.jones.1@bham.ac.uk)

The luminescent hexaalkoxytriphenylene derivatives,<sup>1</sup> triphenoxazoles (**Figure 1a**), combine a large pseudo Stokes shift (**Figure 1b**) and high quantum yield to produce brightly emissive organic fluorophores. Unusually for organic fluorophores the emission wavelength, and Stokes shift, can be dictated through the modulation of group on two position of the oxazole in a predictable manner. To our knowledge the 9 anthryl derivative **TpOx-9-An** exhibits the largest Stokes shift of any organic fluorophore with 377 nm (23700 cm<sup>-1</sup>). As with the parent hexaalkoxytriphenylene,<sup>2,3</sup> triphenoxazoles are thermotropic liquid crystals with columnar hexagonal (col<sub>h</sub>) mesophases (**Figure 1c**) observed, typically > 100 °C. We have observed a red shift in the emission wavelength from a solid sample when heated past the transition into the columnar hexagonal mesophase. This indicates that there is an increased stabilisation of the excited state originating from the close proximity of adjacent molecules in the col<sub>h</sub> mesophase. Additionally triphenoxazoles are photoconductive when irradiated with 350 nm light (**Figure 1d**). The aromatic triphenoxazoles display an increase in current upon irradiation with UV light as well as with increasing temperature, reaching a plateau upon transitioning into the col<sub>h</sub> mesophase. The generation of a photocurrent has highlighted these materials for use in future organic photovoltaics in a similar fashion to other liquid crystalline hexaalkoxytriphenylenes.<sup>4</sup> Within the group both a prototype organic photovoltaic device and prototype organic light emitting diode using **TpOx-2-Nap** as the active layer for both devices. This unique combination of properties has led to the filing of five patents and the subsequent creation of a University of Birmingham spinout company, ChromaTwist Ltd, which is currently looking to bring these materials to the flow cytometry and bio-imaging reagents markets as well towards uses in organic electronic devices.



**Figure 1.** a) Example structure of a triphenoxazole, **TpOx-2-Np** b) Absorption (dashed) and emission (solid) spectra of **TpOx-2-Np** in EtOAc at 10<sup>-5</sup> M c) POM image of **TpOx-2-Np** under crossed polarisers at 184 °C on cooling d) Current generated when an ITO sandwich cell containing **TpOx-2-Np** is illuminated with 350 nm light.

## References

1. UK Pat., WO2019/180445, 2019
2. R. Bushby, Q. Liu, O. Lozman, Z. Lu, S. McLaren, *Molecular Crystals and Liquid Crystals*, 2004, **411**, 293-304.
3. P. Morales, J. Lagerwall, P. Vacca, S. Laschat, G. Scalia *Beilstein Journal of Organic Chemistry*, 2010, **6**, 51.
4. M. Bajpai, N. Yadav, S. Kumar, R. Srivastava, R. Dhar, *Liquid Crystals*, 2016, **43**, 928-936.



# The Design of Novel Liquid Crystal Droplets as Biosensors

Parry, Adele A<sup>1\*</sup>; Paterson, Daniel A<sup>1</sup>; Bao, P<sup>1</sup>; Jones, J Cliff<sup>1</sup>; Peyman, Sally A<sup>1</sup>; Sandoe,

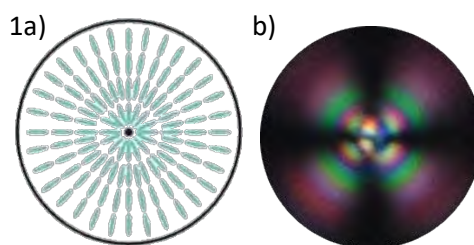
Jonathan<sup>2</sup>; Bushby, Richard<sup>1</sup>; Evans, Stephen D<sup>1</sup> and Gleeson, Helen F<sup>1</sup>

<sup>1</sup>School of Physics and Astronomy, University of Leeds, UK

<sup>2</sup>Leeds Institute of Biomedical and Clinical Science, University of Leeds, UK

Recently, Liquid crystal (LC) droplet research has seen significant interest as a result of their novel applications, including biosensing. The sensitivity of LCs to surface interactions, and the change in anchoring strength which causes changes in the LC's optical properties<sup>1</sup> make them particularly attractive for use as potential biosensors. Further, LCs birefringent properties, mean that an optical signal can be produced with no required labelling of the target biomolecule. The potential for LC droplets to produce inexpensive, sensitive sensors is significant, and therefore makes them extremely interesting to study.<sup>2</sup>

The droplets considered here are produced using flow-focusing microfluidics, and consist of a nematic LC coated in a phospholipid monolayer, with straight chain phospholipids inducing homeotropic (radial) alignment<sup>2</sup>. These lipid-coated droplets are considered as potential mammalian and bacterial cell mimics, with the ability to detect a range of key analytes. We focus on better understanding the stability of such droplets, both as a colloidal suspension and in terms of their alignment state over a 24hr period. Both electrostatic and steric stabilized lipid-coated E7 droplets are considered, with two key lipid combinations being explored: 1,2-Dioleoyl-sn-glycero-3-phosphocholine (DOPC) with 1,2-dioleoyl-sn-glycero-3-phospho-rac-(1-glycerol) sodium salt (DOPG) for electrostatic stabilisation, and DOPC with 1,2-distearoyl-sn-glycero-3-phosphoethanolamine-N-[methoxy(polyethylene glycol)-2000] (ammonium salt) (DSPE-PEG(2000)) for steric stabilisation. Both the overall lipid concentration and compositions of the mixtures are varied, with the resulting alignment and number of droplets/ $\mu$ l described as a function of time.



1) Homeotropic (radial) droplet depicted a) schematically and b) using POM.

**Acknowledgements:** The authors thank: the EPSRC, grant numbers EP/P024041/1, EP/P023266/1 (SDE), and EP/S029214/1 (JCJ). AP is funded by the SOFI CDT.

## References:

[1] T. Cronin, Handbook of Liquid Crystals, J.W Goodby, P.J Collings, T. Kato, C. Tschierske, H.F Gleeson & P. Raynes. Wiley (2014)

[2] P. Bao, D.A. Paterson, P.L Harrison, K. Miller, S. Peyman, J.C Jones, J. Sandoe, S.D. Evans, R.J. Bushby & H.F. Gleeson, Lab-on-a-Chip, (2019)

\* Author for Correspondence: [py14ap@leeds.ac.uk](mailto:py14ap@leeds.ac.uk)

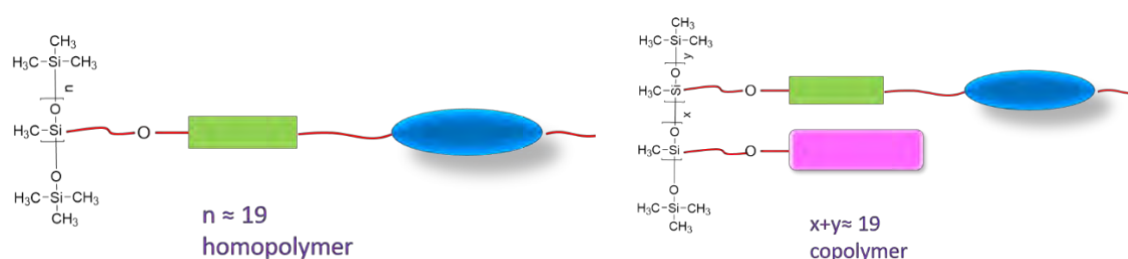
# The investigation of dimeric nematogens linked to polysiloxane main chains

Wanhe Jiang, Georg H. Mehl Department of Chemistry, University of Hull, Hull, HU67RX

The twist-bend nematic phase ( $N_{tb}$ ) is characterised by the spontaneous formation of chiral domains<sup>1-3</sup>. Typically, it is observed in dimers or oligomers, and it can be induced in mixtures<sup>4-5</sup>.

Additionally it can be detected in linear main chain liquid crystal polymers<sup>6-7</sup>. However, the formation of side-chain liquid crystal polymers has not been yet explored to any extent.

Here we report the results of our efforts to synthesize and investigate liquid crystal side-chain polymers which are designed to form the  $N_{tb}$  phase neat or in mixtures. A particular focus is on the design of materials, which form liquid crystal phase behaviour close to room temperature and which show low glass transition temperatures. To achieve this, we decided to employ a siloxane main-chain known to show low glass transition temperatures<sup>8</sup>. We show the synthesis of the monomers in a 14-step synthesis, and discuss the properties of the formed polymers and selected copolymers and mixtures with  $N_{tb}$  dimers, based on optical polarizing microscopy (OPM) and differential scanning calorimetry (DSC) measurements and correlate our results with earlier results.



1. Saha, R. et al.; *Materials Horizons* **2019**, *6*, 1905-1912.
2. Mandle, R. J.; *Soft Matter* **2016**, *12*, 7883-7901.
3. Stevenson, W. D. et al. ; *Physical Chemistry Chemical Physics* **2018**, *20*, 25268-25274.
4. Panov, V. P. et al ; *Crystals* **2021**, *11*, 621.
5. Ramou, E. et al. ; *Liquid Crystals* **2018**, *45*, 1929-1935.
6. Stevenson, W. D. et al. ; *Soft Matter* **2018**, *14*, 3003-3011.
7. Ungar, G. et al.; *Macromolecules* **1992**, *25*, 75-80.
8. Robert, D. et al.; *Journal of the Chemical Society, Chemical Communications* **1990**, 95-97.

# Synthesis and characterisation of a new liquid crystal dimers exhibiting the heliconical twist-bend smectic ( $\text{SmC}_{\text{TB}}$ ) phase.

Gibb, Calum J.<sup>1\*</sup>; Storey, John M.D.<sup>1</sup>; Pocięcha, Damian<sup>2</sup>; Gorecka, Ewa<sup>2</sup> and Imrie, Corrie T.<sup>1</sup>

<sup>1</sup> Department of Chemistry, University of Aberdeen, Aberdeen, UK

<sup>2</sup> Department of Chemistry, University of Warsaw, Warsaw, Poland

In predicting the existence of the now widely studied twist-bend nematic ( $\text{N}_{\text{TB}}$ ) phase, Ivan Dozov also postulated the possibility of a smectic phase which would also contain a short pitch helix.<sup>[1]</sup> Some 20 years later, the first example of a liquid crystal dimer exhibiting the heliconical twist-bend smectic ( $\text{SmC}_{\text{TB}}$ ) phase was discovered.<sup>[2-4]</sup> The  $\text{SmC}_{\text{TB}}$  phase shows many fascinating characteristics but perhaps the most interesting is the formation of a lamella chiral superstructure constructed from achiral molecules.

A library of new materials containing similar structures to the original twist-bend smectogens have been synthesized.<sup>[2]</sup> These molecules exhibit a plethora of fascinating liquid crystalline polymorphism including further examples of the  $\text{SmC}_{\text{TB}}$  phase. They have been characterized using differential scanning calorimetry, polarized optical microscopy, birefringence measurements and X-ray diffraction studies. These studies have led to a greater understanding of the formation of twist-bend nematic and smectic phase, and structure-property relationships are beginning to emerge with respect to the formation of the heliconical smectic phases.

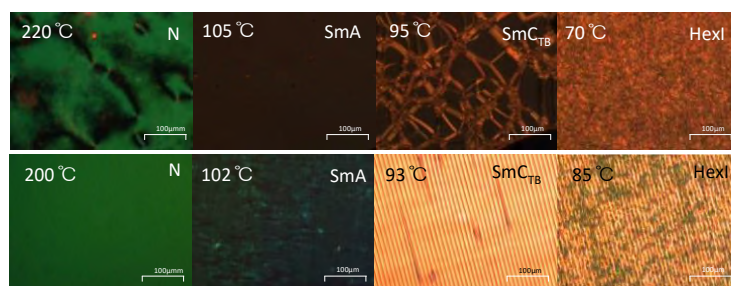


Figure 1: Phase sequence for CB80 CHN OOC O8 viewed between untreated glass slides (top) and in a 1.6 $\mu\text{m}$  aligned cell with planar anchoring (bottom).

## References:

- [1] I. Dozov, *Europhysics Let.*, 56, 247-253 (2001).
- [2] J. P. Abberly, et al, *Nature Commun.*, 9, 228 (2018).
- [3] R. Walker, *Soft Matter*, 15, 3188-3197 (2019).
- [4] M. Salamończyk, et al, *Nature Commum*, 10 (2019)

Author for Correspondence: [c.gibb.18@abdn.ac.uk](mailto:c.gibb.18@abdn.ac.uk)

Helen Gleeson:  
Surprise Surgeon lecture

# Poster Presentations

## **Poster Prize in memory of Mark Warner**

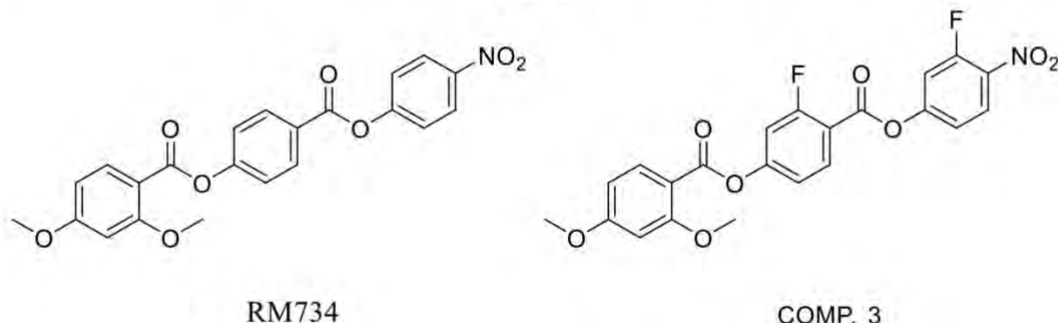
At the British Liquid Crystal Society, he was known for his generosity in sharing knowledge and support, especially with students and young scientists. To celebrate his life and legacy, a member of the BLCS, who would like to stay anonymous, has donated £100 for the Mark Warner Poster Prize which will be given for the poster with the best outreach potential

# P1 The Effect of Fluorination on the Ferroelectric Nematic Phase

Brown, Stevie<sup>1\*</sup>; Cruickshank, Ewan<sup>1</sup>, Storey, John<sup>1</sup>, Imrie, Corrie<sup>1</sup>, Pocięcha, Damian<sup>2</sup>,  
Majewska, Magdalena<sup>2</sup>, Makal, Anna and Gorecka, Ewa

<sup>1</sup>Department of Chemistry, University of Aberdeen, Aberdeen, AB24 3UE, UK

<sup>2</sup>University of Warsaw, Faculty of Chemistry, ul. Zwirki i Wigury 101, 02-089, Warsaw, Poland



**Figure 1** - Chemical structures of RM734 and COMP. 3.

In the conventional nematic phase, the molecules are dispersed randomly along the director,  $\mathbf{n}$ , and show no long-range positional order. The molecules tend to possess chemically distinct ends which are evenly distributed with respect to the director so that the phase shows apolar character i.e  $\mathbf{n} = -\mathbf{n}$ . In 2017, RM734, shown in **Figure 1**, was reported to show a new nematic phase,<sup>[1]</sup> and this was later identified to be the ferroelectric nematic phase.<sup>[2]</sup> The ferroelectric nematic phase, unlike the conventional nematic phase, is polar in nature due the molecular ends aligning in a single direction. The ferroelectric nematic phase is fascinating because it is sensitive to external electric fields and so has properties that make it suitable for use in display devices. Direct isotropic to ferroelectric transitions are very rare with few examples within literature.<sup>[3][4][5]</sup> Here we report other molecules including COMP. 3, **Figure 1**, that show this unusual transition and discuss the effect that fluorination has on the ferroelectric nematic phase.

**Acknowledgements:** This work was financially supported by the Engineering and Physical Sciences Research Council [EP/V048775/1].

## References:

- [1] Mandle, R. J. et al. *Phys. Chem. Chem. Phys.* **19**, 11429–11435 (2017).
- [2] Chen, X. et al. *Proc. Natl. Acad. Sci. U.S.A.* **117**, 14021–14031 (2020).
- [3] Manabe, A. et al. *Liq. Cryst.* **48**, 1079-1086, (2021).
- [4] Jinxing, L. et al. *Chem. Soc.* **143**, 42, 17857–17861 (2021)
- [5] Brown, S. et al. *ChemPhysChem*, **22**, 2506-2510, (2021).

\* Author for Correspondence: [s.brown.19@abdn.ac.uk](mailto:s.brown.19@abdn.ac.uk)

# P2 Synthesis and Characterization of Disulphide- and Thioether-linked Liquid Crystal Dimers

Tufaha, Naila\*; Gibb, Calum J; Imrie, Corrie T and Storey, John MD<sup>1</sup>

<sup>1</sup> Department of Chemistry, University of Aberdeen, Aberdeen, United Kingdom

The dependence of the transitional behaviour of liquid crystal dimers on their molecular structure has been the focus of considerable research activity in recent years. Much of this work has centred on the twist bend phases. [1][2] In order to control the bend of these dimers, various oxygen functionalities have been employed as linkers for the flexible spacers. Sulfur-containing materials have not been investigated to the same extent, but it has been reported that the introduction of the C-S-C link, having a more acute bond angle than the corresponding C-C-C and C-O-C links, influences the temperature range of the mesophases observed. [3][4] The highly polarizable nature of sulfur atoms enhances the birefringence of these materials which is of great interest in developing liquid crystal display technologies. [5][6][7]

Here we present the synthesis and characterization of a series of dimers linked by a disulphide bridge (Figure 1). In addition, we also present examples of thioether-linked dimers and discuss the role that these sulfur links have in the formation of the  $N_{TB}$  phase.

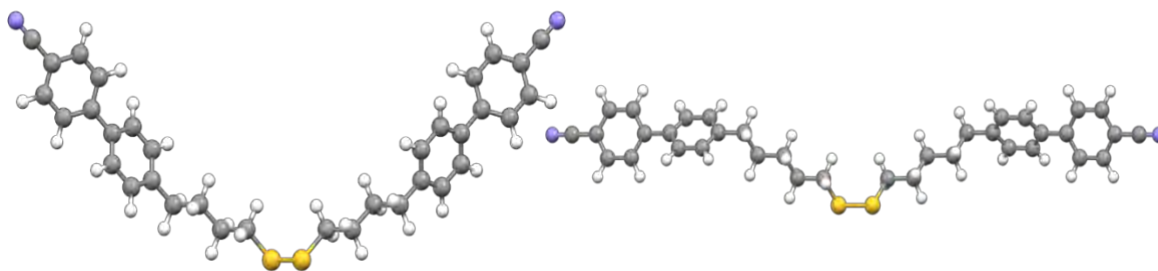


Figure 1 - Molecular models of members of the CBnSSnCB series.

## References:

- [1] E. Cruickshank, et al., *Liq. Cryst.*, **46**, 10 (2019).
- [2] Z. Fang, C. Wu, *Liq. Cryst.*, **47**, 7, 1086-1099 (2020).
- [3] Y. Arakawa, et al., *Chem. Eur. J.*, **26**, 3767-3775 (2020).
- [4] Y. Arakawa, et al., *J. Molec. Struct.*, **1199**, 126913 (2020).
- [5] M. Mansueto, et al., *Tetrahedron*, **70**, 36, 6258-6264 (2014).
- [6] D. Bruce, et al., *Comprehensive Organometallic Chemistry III*, **12**, 195-293 (2007).
- [7] C.T. Imrie, P.A. Henderson, *Chem. Soc. Rev.* **36**, 12, 2096-2124 (2007).

\* Author for Correspondence: [n.tufaha21@abdn.ac.uk](mailto:n.tufaha21@abdn.ac.uk)

# Strain Induced Changes in Order and the Auxetic Response in a Liquid Crystal Elastomer

Aidan Street<sup>1</sup>, Thomas Raistrick, Zhaopeng Zhang & Helen F Gleeson  
*School of Physics and Astronomy, University of Leeds, Leeds, LS2 9JT, UK*

Liquid crystal elastomers (LCEs) are crosslinked polymers, they exhibit properties such as rubber-like elasticity and the anisotropy that usually characterises liquid crystals. A property that has been recently observed in LCEs is an auxetic response [1]. Auxetic materials where the Poisson's ratio is negative are much sought after however the mechanism for the auxetic response is yet to be fully explained [2].

The order in a new, lightly crosslinked liquid crystal elastomer, related to that reported in [1] was examined via the polarised Raman spectroscopy (PRS) method described in detail by Southern & Gleeson [3] to assess the order parameters (OPs) and how they depend on mechanical deformation perpendicular to the unstrained nematic director.

Initially, the uniaxial OPs  $\langle P200 \rangle$  and  $\langle P400 \rangle$  take values at 0.60 and 0.31 before quickly reducing to zero where a mechanical Fréedericksz transition (MFT) occurs, in the MFT the director reorients to align itself parallel to the strain axis. It is in this region that the auxetic behaviour appears and the Poisson's ratio is seen to be negative where expansion occurs in a direction perpendicular to the applied strain.

At low strains, the LCE showed behaviour consistent with the theoretical predictions of Maier-Saupe theory. However, as strain increases towards the MFT,  $\langle P200 \rangle$  reduces faster than  $\langle P400 \rangle$  which is not in agreement with the Maier-Saupe predictions. This deviation from the theoretical predictions is explained by the emergence of the biaxial order parameters,  $\langle P220 \rangle$ ,  $\langle P420 \rangle$  and  $\langle P440 \rangle$ .

The emergence of biaxial order and the auxetic response of this system are compared to the previously reported LCE.

## References

- [1] D. Mistry, S. D. Connell, S. L. Mickthwaitee, P.B. Morgan, J. H. Clamp & H. F. Gleeson, Coincident molecular auxeticity and negative order parameter in liquid crystal elastomer, *Nat Commun* 9, 5095 (2018)
- [2] T. Raistrick, Z. Zhang, D. Mistry, J. Mattson and H. F. Gleeson, Understanding the physics of the auxetic response in a liquid crystal elastomer, *Phys. Rev. Research* 3, 023191
- [3] C. D. Southern and H. F. Gleeson Using the full Raman depolarisation in the determination of the order parameters in liquid crystal systems *Eur. Phys. J. E* 24, 119-127 (2007)

---

<sup>1</sup> py18ajs@leeds.ac.uk



Iman Zulkhairi<sup>1</sup>, Ivan Dominguez-Candela<sup>1,2</sup>, Inmaculada Pintre<sup>3</sup>, M. Blanca Ros<sup>3</sup>, Alfonso Martinez-Felipe<sup>1,4</sup>

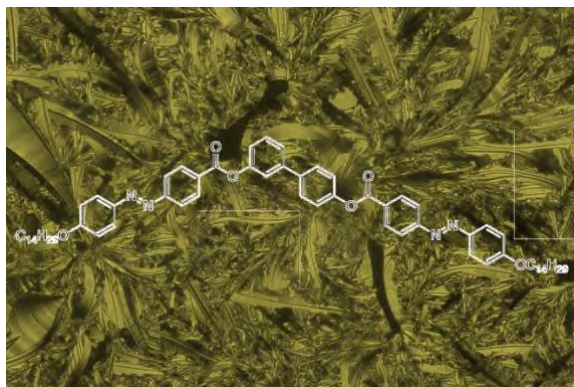
<sup>1</sup>Chemical Process and Materials Research Group, School of Engineering, University of Aberdeen, King's College, Aberdeen AB24 3UE, Scotland, UK

<sup>2</sup>Instituto de Seguridad Industrial, Radiofísica y Medioambiental (ISIRYM) Universitat Politècnica de València (UPV), Plaza Ferrándiz y Carbonell, s/n 03801 Alcoy, Spain

<sup>3</sup>Instituto de Nanociencia y Materiales de Aragón, Departamento de Química Orgánica, Facultad de Ciencias, Universidad de Zaragoza-CSIC, Campus San Francisco, E-50009 Zaragoza, Spain.

<sup>4</sup>Centre for Energy Transition, University of Aberdeen, King's College, Aberdeen AB24 3UE, Scotland, UK.

The energy transition towards net-zero societies requires explorations on alternative power generation and energy storage methods based on renewable resources. Liquid crystals have attracted great interest in advanced applications, including in energy devices, due to their response to external stimuli, and their capacity to form controlled nanostructures<sup>1</sup>. Their anisotropy can be used, for example, to store energy (in ferroelectric materials)<sup>2</sup>, and also to transfer charges efficiently (through oriented polar channels)<sup>3</sup>. In this work we assess the potential as energy harvesters of a series of photoresponsive bent-core materials containing azobenzene groups capable to undergo *trans-to-cis* photoisomerisation by UV irradiation. The materials show smectic and columnar phases ( $SmC_aP_a$ ,  $SmA$  and  $Col_{ob}$ )<sup>4</sup>, which are evaluated under the presence of electrical fields (up to  $250 \text{ kV}\cdot\text{cm}^{-1}$ ) and UV illumination (up to  $1000 \text{ mW}\cdot\text{cm}^{-2}$ ). Their dielectric relaxations have been also studied by using impedance spectroscopy in a wide range of frequencies (0.01 to  $10^6$  Hz), as a function of the temperature. By performing current-voltage hysteresis loops, we have determined their macroscopic polarization, and their tendency for relaxor ferroelectric behaviour. Our results can lead towards the preparation of energy harvesters triggered by light-irradiation, with the potential to store energy from renewable sources.



Banana-leaf texture associated to the formation of columnar mesophases by an azobenzene bent-core material (T=144°C)

### References

1. Fitzgerald, R. J., 2018. The nature and art of liquid crystals. *Physics Today*, 71(10), p. 76.
2. Takezoe, H. & Takanishi, Y., 2006. Bent-core liquid crystals: their mysterious and attractive world. *Japanese Journal of Applied Physics*, 45(2A), pp. 597-625.
3. Alaudin et al., 2021, New side-chain liquid crystalline terpolymers with anhydrous conductivity: Effect of azobenzene substitution on light response and charge transfer *European Polymer Journal*, 146, p. 110246.
4. Pintre I.C. et al. Liquid crystalline and nonlinear optical properties of bent-shaped compounds derived from 3,49-biphenylene, *J Mater Chem*, **2007**, 17, 2219–2227.

Noor Zahra<sup>1</sup>, Daniel Zaton<sup>1,2</sup>, Alexia Karamoula<sup>1</sup>, John M.D. Storey<sup>2</sup>, Corrie T. Imrie<sup>2</sup>, Alfonso Martinez-Felipe<sup>1,3</sup>

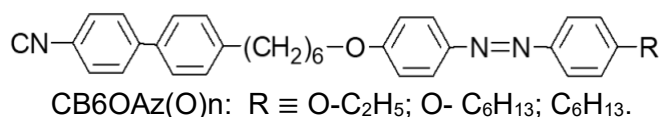
<sup>1</sup>Chemical Process and Materials Research Group, School of Engineering, University of Aberdeen, King's College, Aberdeen AB24 3UE, Scotland, UK.

<sup>2</sup> Department of Chemistry, School of Natural and Computing Sciences, King's College, University of Aberdeen, Aberdeen, AB24 3UE, UK.

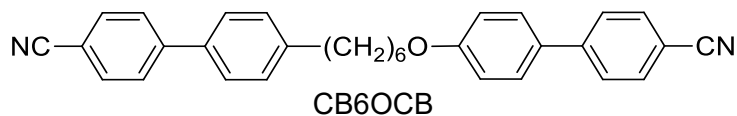
<sup>3</sup>Centre for Energy Transition, University of Aberdeen, King's College, Aberdeen AB24 3UE, Scotland, UK.

The twist-bend nematic,  $N_{TB}$ , phase can be considered as a generalised case of the chiral nematic phase,  $N^*$ , with the director,  $n$ , simultaneously twisting and bending. In the resulting nanoscale consisting of helical structures,  $n$  is tilted at a constant angle  $\theta < 90^\circ$  with respect to the helix axis<sup>1,2</sup>. The  $N_{TB}$  phase is locally chiral, even though it is composed of achiral molecules, and represents the first example of spontaneous chiral symmetry breaking in a fluid system with no long-range positional order. Since its experimental discovery in 2011<sup>3</sup>, the  $N_{TB}$  phase continues to attract interest, from both fundamental and applied grounds. More specifically, the introduction of chromophores offers a very attractive way to exert spatial control over the properties and functionalities of new  $N_{TB}$  materials<sup>4</sup>.

We have recently described the phase behaviour and light response of a series of non-symmetric dimers including cyanobiphenyl and azobenzene groups, linked by flexible hexyloxy spacers. The so-called  $CB6OAz(O)n(s)$  exhibit conventional N and  $N_{TB}$  phases, modulated by light irradiation<sup>5</sup>,



We now explore the phase behaviour and UV response of mixtures of our  $CB6OAz(O)n(s)$  dimers with the archetypal  $N_{TB}$  host 1-(4-cyanobiphenyl-4-yloxy)-6-(4-cyanobiphenyl-4-yl)hexane,  $CB6OCB$ ,



We have performed a detailed dielectric analysis of  $CB6OCB / CB6OAz(O)n(s)$  mixtures, containing 5% of azobenzene molecules (molar %), using impedance spectroscopy in a wide range of frequencies (0.01 to 10<sup>6</sup> Hz), and as a function of the temperature. We have also evaluated their ferroelectric response, by performing current-voltage hysteresis loops. Our results can lead towards the preparation of new functional materials exhibiting the  $N_{TB}$  phase, based on light sensing or harvesting.

## References

1. Meyer R. R. Balian, G. Weil, editors. *Molecular fluids*. New York: Gordon and Breach; **1976**.
2. Dozov I. On the spontaneous symmetry breaking in the mesophases of achiral banana-shaped molecules. *Europhys Lett* **2001**, 56, 247.
3. Cestari M et al. Phase behavior and properties of the liquid-crystal dimer 1',7'-bis(4-cyanobiphenyl-4'-yl) heptane: A twist-bend nematic liquid crystal. *Phys Review E* **2011**, 16, 84.
4. Paterson, D. et al. Azobenzene-Based Liquid Crystal Dimers and the Twist-Bend Nematic Phase. *Liq Cryst* **2017**, 44, 2060–2078.
5. Zaton et al. Photo-driven effects in twist-bend nematic phases: Dynamic and memory response of liquid crystalline dimers. *J Mol Liq* **2021**, 344, 117680.

## Experimental and Computational Studies of the Effect of Molecular Design on Smectic A Liquid Crystal Phases

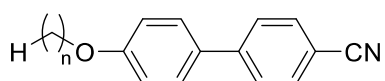
Giuseppina Barile, Laurence C. Abbott, Stephen J. Cowling, John N. Moore

Department of Chemistry, University of York, Heslington, York, YO10 5DD

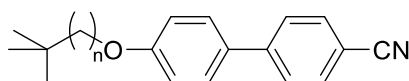
Smectic A liquid crystal phases exhibit both orientational and translational order, leading to a phase structure of diffuse layers with a molecular director that is perpendicular to the layer plane. Smectic A materials can be used in a wide range of applications such as guest-host devices and smart windows, and within devices that can provide favourable properties, such as low power consumption or high contrast.

The molecular design used to provide liquid crystal phases is important to ensure the optimisation of favourable properties and much work has focussed on the use of terminal groups to favour the formation of the smectic A phase through nanophase segregation. Many different terminal groups such as siloxanes,<sup>1</sup> have been found to induce the organisation of the molecules into segregated layers. Previous work has also found that the tBu terminal group also gives rise to this effect, notably in comparison with a straight chain analogue.<sup>2</sup>

In this work, we have been probing the effect of bulky terminal groups through combined experimental and computational studies of the n-alkoxycyanobiphenyl (nOCB) and the tBu-n-alkoxycyanobiphenyl (tBu-nOCB) series, as shown below.



nOCB, where n = 8-13



tBu-nOCB, where n = 6-11

The experimental work has used polarised optical microscopy to characterise the phases present, and X-ray diffraction measurements have probed the layer spacing observed for the smectic A phase for the two series of molecules. These methods have given an insight into the effect of the tBu group on the phases observed and on how this group affects the layered structure of the phase. Fully atomistic molecular dynamic simulations have been used to model the two series and give comparisons with the experimental results, thereby providing additional understanding of the phases formed. Further work involves guest-host systems containing anthraquinone dyes, including studies into the effects of molecular design of both host liquid crystal and guest dye molecules.

1. R. J. Mandle, E. J. Davis, C. C. A. Voll, D. J. Lewis, S. J. Cowling and J. W. Goodby, *Journal of Materials Chemistry C*, 2015, **3**, 2380-2388.
2. M. T. Sims, L. C. Abbott, J. W. Goodby and J. N. Moore, *Soft Matter*, 2019, **15**, 7722-7732.

## Mathematical modelling of antibiotic tolerance in liquid crystalline biofilms

Maria Tessel van Rossem<sup>1\*</sup>, Sandra Wilks<sup>1</sup>, Malgosia Kaczmarek<sup>1</sup>; Patrick Secor<sup>2</sup>; Giampaolo

D'Alessandro<sup>1</sup>

<sup>1</sup> University of Southampton, Southampton, UK

<sup>2</sup>University of Montana, Missoula, Montana, USA

Antibiotic resistance and tolerance in bacteria are serious medical issues of strong scientific interest. Recently, Patrick Secor et al. discovered liquid crystalline order in *Pseudomonas aeruginosa* biofilms, which was found to lead to increased antibiotic tolerance [1]. These liquid crystals are formed by the filamentous bacteriophage Pf4 in combination with polymers in the biofilm matrix, through an excluded volume effect termed depletion attraction. The modelling of biofilms is generally limited to cell-level simulations and population dynamics, and no continuum models of liquid crystalline biofilms exist. We aim to work towards the development of such models to explain the contribution of liquid crystalline order in biofilms to antibiotic tolerance and resistance.

A simplified *in vitro* model of Pf4 virion-induced liquid crystals consists of suspensions of Pf4 virions and depleting polymers, with the bacteriophages forming liquid crystalline droplets called tactoids. These tactoids encapsulate bacteria, forming a protective barrier against cationic antibiotics through adsorption by the anionic bacteriophages. We investigate if this barrier can be effective through physical mechanisms alone, by adsorption and impeded diffusion. To this end we have developed a numerically solvable continuum model of the diffusion of antibiotics through a tactoid. We have also developed an effective, analytically solvable model using the mathematical technique of homogenisation, to gain additional insight into the significance of the problem parameters.

Our results show that the tactoid barrier has a significant effect on the diffusion of antibiotics, and that the ability of the bacteriophages to adsorb antibiotics is essential for this efficacy. This agrees with previous experimental findings which show that the presence of Pf4 virions only increases tolerance to cationic antibiotics [1][2]. The developed model sets a step towards the modelling of liquid crystalline biofilms in their full complexity. In particular, the effective homogenised model is straightforwardly extendable to more complex geometries. In parallel to modelling, we carry out experiments to grow and characterise liquid crystalline phage suspensions. We plan to use these experiments to validate the conclusions of our mathematical model. Ultimately, we hope to contribute useful insights into the structure of biofilms and the treatment of bacterial infections.

### References:

[1] P. R. Secor et al., *Cell Host Microbe*, **18**, 5 (2015).

[2] A. K. Tarafder et al., *Proc Natl Acad Sci USA*, **117**, 9 (2020).

# P8 Accurate modelling of liquid crystal devices including diffractive effects.

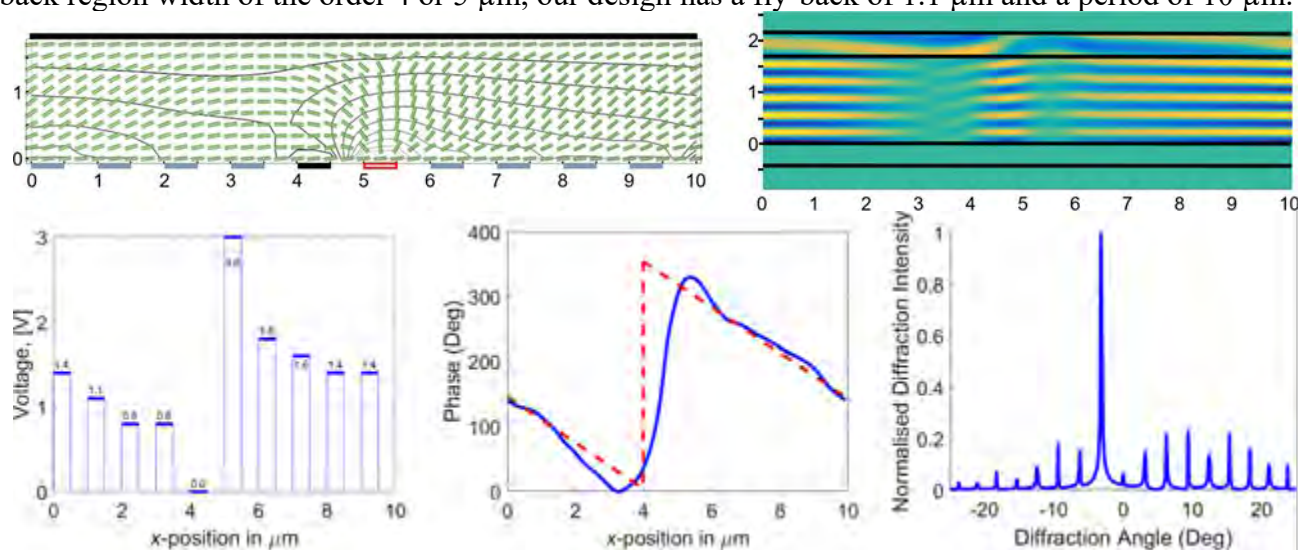
Dezhi Shen<sup>1</sup>, Mengyang Yang<sup>2</sup>, F. Anibal Fernandez<sup>1</sup>

<sup>1</sup>University College London, London, United Kingdom, <sup>2</sup>Microsoft Research Cambridge, Cambridge, United Kingdom.

## Abstract

We present an accurate method to study the optical behaviour of liquid crystal (LC) devices. The method is particularly applicable to devices containing small features or where LC defects are present. The procedure combines an accurate LC modelling with a full-field electromagnetic solver, both specially written for LC devices. The LC modelling is based on the Landau- DeGennes theory combined with Sonnet *et al.* approach for the LC hydrodynamics [1,2] and is implemented using finite elements [3,4]. The electromagnetic modelling takes full account of the non-uniformity and anisotropy of the LC permittivity distribution obtained from the order tensor. It is based on the total field / scattered field approach to electromagnetic scattering problems, implemented as a finite differences in the frequency domain (FDFD) approach. Open boundaries are modelled using the stretched coordinates formulation of perfectly matched layers and the resultant matrix problem is solved using GMRes with an especially adapted form of a sweeping preconditioner. Although the methods are all applicable to 3D problems, the preconditioner, needed for an efficient solution, so far has only been implemented in 2D.

The modelling procedure is demonstrated here with a novel design of an LC blazed phase grating where defects are deliberately introduced in order to obtain an abrupt fly-back. While a conventional LCOS gratings, with a small pixel pitch of 4  $\mu\text{m}$  and ten levels of phase, would have a period of 40  $\mu\text{m}$  and a fly-back region width of the order 4 or 5  $\mu\text{m}$ , our design has a fly-back of 1.1  $\mu\text{m}$  and a period of 10  $\mu\text{m}$ .



- [1] AM Sonnet and EG Virga, Phys Rev E, 2001;64:031705.
- [2] AM Sonnet, PL Maffettone and EG Virga, J Non-Newtonian Fluid Mech, 2004;119:51-59.
- [3] EJ Willman, FA Fernández, R James and SE Day, IEEE Trans Electron Devices, 2007; 54(10): 2630-2637.
- [4] R James, EJ Willman, FA Fernández and SE Day, IEEE Trans Magn, 2008;44(6):814-817.

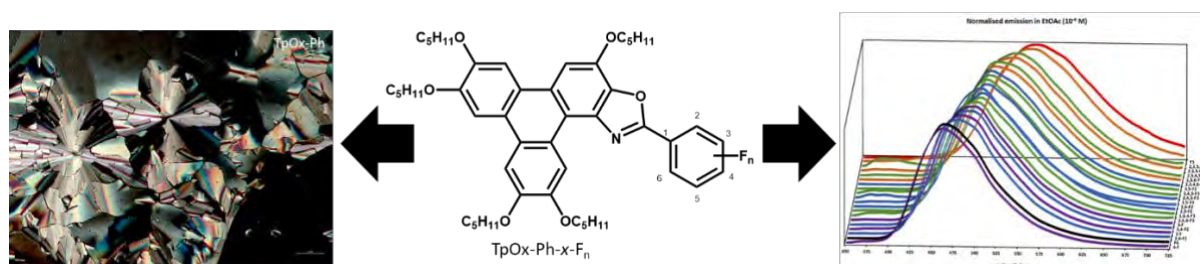
Michael S. Butlin<sup>1</sup>, Gregory C. O'Callaghan<sup>1</sup>, Owen M. Jones<sup>1</sup>, Karolis Viržbickas<sup>2</sup>, Dennis Zhao<sup>1</sup>, Alexander P. G. Robinson<sup>2</sup> and Jon A. Preece<sup>1</sup>

<sup>1</sup> School of Chemistry, University of Birmingham, UK, B15 2TT

<sup>2</sup> School of Chemical Engineering, University of Birmingham, UK, B15 2TT

\*[mxb385@student.bham.ac.uk](mailto:mxb385@student.bham.ac.uk)

Triphenoxazoles are hexalkoxytriphenylene based organic dye molecules with large *pseudo* Stokes shifts and high brightness.[1] A series of 19 fluorophenyl functionalised triphenoxazoles (TpOx-Ph-x-F<sub>n</sub> – Figure 1) were synthesised for the purpose of examining the effect of electron withdrawing group substitution pattern on the triphenoxazole emission spectrum. The *pseudo* Stokes shift was found to correlate strongly with the Hammett constant of the parent fluorobenzoic acid [2] leading to predictive power when designing new emissive dyes.



The **Figure 4.** The fluorophenyl triphenoxazoles (TpOx-Ph-x-F<sub>n</sub>) form col<sub>h</sub> phases (POM image - left) and emit across the visible region (right)

thermotropic liquid crystalline properties of the materials were characterised by Polarising Optical Microscopy (POM – Figure 1) and Differential Scanning Calorimetry (DSC) showing the series was typically liquid crystalline >90 °C. A columnar hexagonal (col<sub>h</sub>) phase then persisted to approx. 300 °C for several of the compounds studied.

In 2018 triphenoxazoles were commercialised through the formation of University of Birmingham spinout company; ChromaTwist LTD, with the company recently named “one to watch” by the Nature Research Spinoff Prize 2020. Ultimately the triphenoxazoles may find applications in the fields of life sciences or organic electronics.

#### References

[1] UK Pat., WO2019/180445, (2019).

[2] W. Kosaka, M. Itoh and H. Miyasaka, *Dalton T.*, **44**, 8156-8168, (2015).

## New patterns of twist-bend liquid crystal phase behaviour

Walker, Rebecca<sup>1\*</sup>; Alshammari, Ahlam<sup>1</sup>; Cruickshank, Ewan<sup>1</sup>; Pociecha, Damian<sup>2</sup>; Storey, John MD<sup>1</sup>;

Gorecka, Ewa<sup>2</sup> and Imrie, Corrie T<sup>1</sup>

<sup>1</sup> Department of Chemistry, University of Aberdeen, Aberdeen, United Kingdom

<sup>2</sup> Department of Chemistry, University of Warsaw, Warsaw, Poland

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

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

### References:

- [1] I. Dozov, *Europhys. Lett.* **2001**, *56*, 247–253.
- [2] R. B. Meyer, in *Les Houches Summer Sch. Theor. Physics, Mol. Fluids*, Gordon And Breach, New York, **1976**, pp. 316–320.
- [3] V. Borshch, Y. K. Kim, J. Xiang, M. Gao, A. Jáklí, V. P. Panov, J. K. Vij, C. T. Imrie, M. G. Tamba, G. H. Mehl, O. D. Lavrentovich, *Nat. Commun.* **2013**, *4*, 2635.
- [4] J. P. Abberley, R. Killah, R. Walker, J. M. D. Storey, C. T. Imrie, M. Salamończyk, C. Zhu, E. Gorecka, D. Pociecha, *Nat. Commun.* **2018**, *9*, 228.
- [5] M. Salamończyk, N. Vaupotič, D. Pociecha, R. Walker, J. M. D. Storey, C. T. Imrie, C. Wang, C. Zhu, E. Gorecka, *Nat. Commun.* **2019**, *10*, 1922.
- [6] S. P. Sreenilayam, Y. P. Panarin, J. K. Vij, V. P. Panov, A. Lehmann, M. Poppe, M. Prehm, C. Tschierske, *Nat. Commun.* **2016**, *7*, 1–8.

\* Author for Correspondence: [rebecca.walker@abdn.ac.uk](mailto:rebecca.walker@abdn.ac.uk)

Umama Bendaoud<sup>1</sup>, Pradip K. Bhowmik<sup>2</sup>, Omar Noori<sup>2</sup>, Si L. Chen<sup>2</sup>, Haesook Han<sup>2</sup>, Michael R. Fisch<sup>3</sup>, Christina M. Robb<sup>4</sup>, Javier Vergara<sup>5</sup>, M. Blanca Ros<sup>5</sup>, Alfonso Martinez-Felipe<sup>1,6</sup>

<sup>1</sup> Chemical Process and Materials Research Group, School of Engineering, University of Aberdeen, King's College, Aberdeen AB24 3UE, Scotland, UK.

<sup>2</sup> Department of Chemistry and Biochemistry, University of Nevada Las Vegas, 4505 S. Maryland Parkway, Box 454003, Las Vegas, NV 89154, USA.

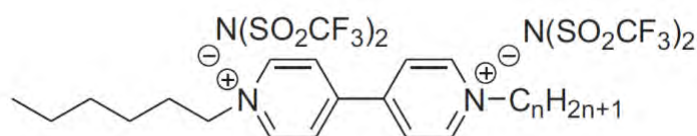
<sup>3</sup> College of Aeronautics and Engineering, Kent State University, Kent, OH 44242, USA.

<sup>4</sup> Department of Chemistry, Kent State University, Kent, OH 44242, USA.

<sup>5</sup> Instituto de Nanociencia y Materiales de Aragón, Departamento de Química Orgánica, Facultad de Ciencias, Universidad de Zaragoza-CSIC, Campus San Francisco, E-50009 Zaragoza, Spain.

<sup>6</sup> Centre for Energy Transition, University of Aberdeen, King's College, Aberdeen AB24 3UE, Scotland, UK.

Ionic liquids (ILs) are salts consisting of organic cations and inorganic/organic anions having melting transitions ( $T_m$ ) lower than 100°C. The presence of rod-like groups can contribute to form mesophases, leading to Ionic Liquid Crystals, ILC, with potential application in a variety of modern fields, including solvents, catalysts, pharmaceutical ingredients, and electrolytes<sup>1</sup>. In this work, we report the conductivity of a series of viologens, containing 4,4'-bipyridinium cores and triflimide anions<sup>2</sup>, which form smectic T phases,



The 6BPn viologens studied in this work, with  $n$  ranging from 5 to 20

We have measured the dielectric response and conductivity of our ILC in a broad range of frequencies and temperatures, reaching direct current conductivities in the  $\sigma_{dc} \sim 10^{-4.5} \text{ S} \cdot \text{cm}^{-1}$  range, which are comparable to other ionic salts studied recently<sup>3</sup>. In addition, we have doped the 6BPn viologens with different molecules containing azobenzene groups, resulting in light-responsive ILC. This strategy yields new electrolytes with conductivity enhanced by light irradiation, which will be further developed into materials for advanced energy applications.

## References

1. Kar, M. et al. Ionic liquids - further progress on the fundamental issues. *Aust J Chem* **2019**, *72*, 3.
2. Bhowmik, P. K. et al. Ionic liquid crystals: Synthesis and characterization via NMR, DSC, POM, X-ray diffraction and ionic conductivity of asymmetric viologen bistriflimide salts. *J Mol Liq* **2021**, *328*, 115370.
3. Bhowmik, P. K. et al. Dicationic stilbazolium salts: structural, thermal, optical, and ionic conduction properties. *J Mol Liq* **2021**, *341*, 117311.