UNIVERSITY OF
BIRMINGHAM

The 2025 British Liquid Crystal Society Annual Meeting and Workshop

Monday 7 – Thursday 10 April 2025

Abstract Book

BLCS2025

Contents

BLCS2025: Welcome Message

On behalf of the British Liquid Crystal Society (BLCS), I am delighted to welcome you to the 2025 BLCS Annual Meeting and Workshop (BLCS2025) at the University of Birmingham.

The BLCS Annual Meeting welcomes researchers from all career stages across all areas of liquid crystals research but is especially aimed at providing a platform for early career researchers – PhD students as well as postdoctoral researchers – so that they can present their work to an expert audience. Alongside the Annual Meeting, a Workshop is being held to provide education and training for the next generation of researchers in the highly interdisciplinary field of liquid crystals research by experts of the field.

It is a pleasure to have this year’s Sturgeon Lecturer, the 2024 and 2025 Gray Medal Lecturers, three Invited Speakers, this year’s Hilsum Medal Winner and BLCS Young Scientist Awardee at the BLCS2025, alongside some more established members of our community. Some of them have kindly agreed to deliver lectures at the Workshop so that we can continue with the tradition of holding a training focused Workshop in the BLCS calendar.

I would like to thank everyone for their participation in the BLCS2025 and/or contribution to its organisation. In particular, I would like to thank our sponsors

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Materials Advances

Soft Matter

MATERIALS CHEMISTRY
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and those who have helped organise the BLCS2025:

The Scientific Committee: Dwaipayan Chakrabarti (Chair), Rebecca Walker and Nigel Mottram;
The Registration Team: Adam Walker and Euan Pattinson

Finally, I would like to gratefully acknowledge support from the University’s Conference and Events Team and Edgbaston Park Hotel & Conference Centre Team, especially Rebecca Amos, Louise Walczak and Tori Smith.

I am looking forward to seeing you at the BLCS2025 and the weather should be a bonus!

Warmly,

Dwaipayan Chakrabarti

Campus Map

Edgbaston Campus Map

Red Zone
R0 The Harding Building
R1 Law Building
R2 Frankland Building
R3 Hills Building
R4 Aston Webb – Lapworth Museum
R5 Aston Webb – B Block
R6 Aston Webb – Great Hall
R7 Aston Webb – Student Hub
R8 Physics West
R9 Nuffield
R10 Physics East
R11 Medical Physics
R12 Bramall Music Building
R13 Poynting Building
R14 Barber Institute of Fine Arts
R15 Watson Building
R16 Arts Building
R17 Ashley Building
R18 Strathcona Building
R19 Education Building
R20 J G Smith Building
R21 Muirhead Tower
R23 University Centre
R24 Staff House
R26 Geography
R27 Biosciences Building
R28 Murray Learning Centre
R29 The Alan Walters Building
R30 Main Library
R31 Collaborative Teaching Laboratory
R32 Teaching and Learning Building
R33 Fry Building
R34 Cuore

Blue Zone
B1 Medical School
B2 Institute of Biomedical Research including IBR West
B3 Wellcome Clinical Research Facility
B4 Robert Aitken Institute for Clinical Research
B5 CRUK Institute for Cancer Studies and Denis Howell Building
B6 Research Park
B7 90 Vincent Drive
B8 Henry Wellcome Building for Biomolecular NMR Spectroscopy
B9 Medical Practice and Dental Centre
B10 Advanced Therapies Facility
B11 BioHub Birmingham
B12 Health Sciences Research Centre (HSRC)

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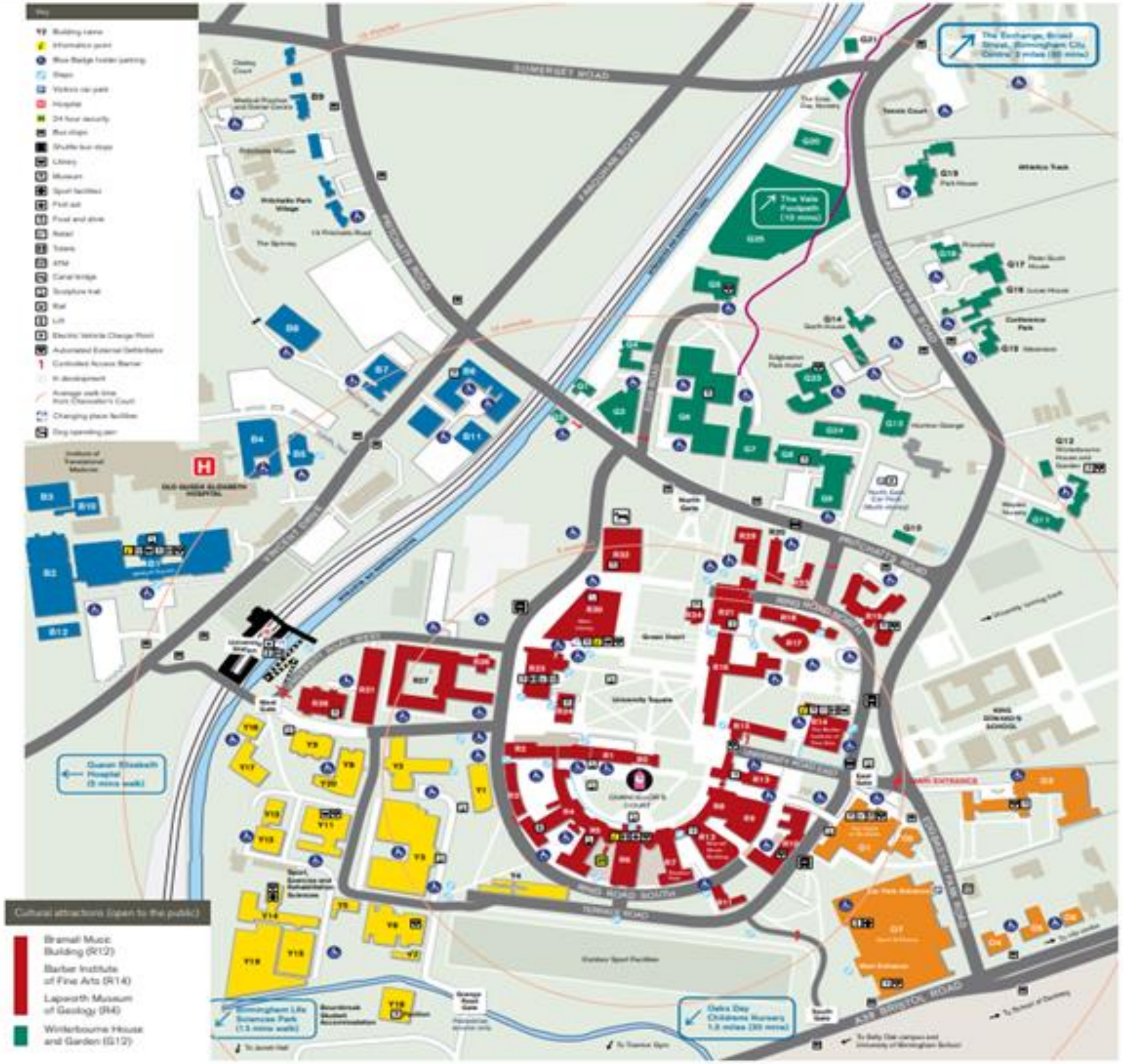
Orange Zone
O1 The Guild of Students
O2 St Francis Hall
O3 University House
O4 Ash House
O5 Beech House
O6 Cedar House
O7 Sport & Fitness

Green Zone
G1 32 Pritchatts Road
G2 31 Pritchatts Road
G3 European Research Institute
G4 3 Elms Road
G5 Computer Centre
G6 Metallurgy and Materials
G7 IRC Net Shape Laboratory
G8 Gisbert Kapp Building
G9 52 Pritchatts Road
G10 54 Pritchatts Road – Institute for Global Innovation
G11 Maples Nursery
G12 Winterbourne House and Garden
G13 Hornton Grange
G14 Garth House
G15 Westmere
G16 Lucas House
G18 Priorsfield
G19 Park House
G20 Wolfson Advanced Glasshouses
G22 Elms Day Nursery
G23 Edgbaston Park Hotel and Conference Centre
G24 Centre for Human Brain Health
G25 EcoLab

Yellow Zone
Y1 The Old Gym
Y2 Haworth Building
Y3 Engineering Building
Y4 Terrace Huts
Y5 Estates West
Y6 Maintenance Building
Y7 Grounds and Gardens
Y8 The School of Engineering
Y9 Computer Science
Y11 Chemical Engineering
Y12 Biochemical Engineering
Y13 Chemical Engineering Workshop
Y14 Sport, Exercise and Rehabilitation Sciences
Y15 Civil Engineering Laboratories
Y16 Institute of Occupational and Environmental Medicine
Y17 Public Health
Y18 Bournbrook Student Accommodation
Y19 NBIF
Y20 UKRRIN



Cultural attractions (open to the public)
🟥 Bramall Music Building (R12)
🟥 Barber Institute of Fine Arts (R14)
🟥 Lapworth Museum of Geology (R4)
🟩 Winterbourne House and Garden (G12)

Useful Information

Venue

The BLCS2025 will be held in the Edgbaston Park Hotel & Conference Centre at the University of Birmingham. The information about travelling to the BLCS2025 venue can be found at https://uobevents.eventsair.com/british-liquid-crystal-society/. The Workshop lectures on Monday the 7th April will take places in the Bantock room in the Edgbaston Park Hotel; the talks for the next three days will be held in the Lloyd Suite (Hornton Grange) and poster presentation will take place in the lounge of the Hornton Grange.

Presentations

Talks: There are 60-minute slots for named/medal Lectures, 45-minute slots for Invited Talks, a 30-minute slot for the BLCS Young Scientist Awardee, and 20-minute slots for Contributed Talks, all including time for questions and answers. There are two 10-minute talks by the sponsors on Tuesday afternoon.

Posters: Poster boards are double sided, and each side should be sufficient for an A0 poster in portrait orientation. The poster boards will be available throughout the day on Tuesday and Wednesday, but there is a dedicated slot for poster presentation on Tuesday evening.

Catering

Refreshments and lunch will be provided on all four days (or on three days for those who opted out of the Workshop) and will be served either in the restaurant of the Edgbaston Park Hotel or in the ground floor of the Hornton Grange. There is no provision for dinner on Monday the 7th and Tuesday the 8th April, but are many restaurants located close by and across the city for you to explore!

There will be a Conference Dinner on Wednesday the 9th evening and is included in your registration, unless you have indicated that you will not attend it. The Conference Dinner will be held in the Lloyd Suite (Hornton Grange).

The BLCS2025 Programme

Day 1: Monday 7 April, Bantock Room

12:15 – 13:45	Registration and Lunch
	The 2025 BLCS Annual Training Workshop Supported by the Royal Society of Edinburgh (RSE)
13:45 – 14:00	Opening Remarks – I
14:00 – 15:00	**Continuum Theories for Liquid Crystals and their Applications** *Apala Majumdar, University of Strathclyde*
15:00 – 16:00	**Computer Simulations of Liquid Crystals** *Mark R. Wilson, Durham University*
16:00 – 16:30	Tea / Coffee Break
16:30 – 17:30	**Structures of Low Molar Liquid Crystals & Liquid Crystal Polymers** *Georg H. Mehl, University of Hull*

Day 2: Tuesday 8 April, Lloyd Suite (Hornton Grange)

	The 2025 BLCS Annual Training Workshop Supported by the Royal Society of Edinburgh (RSE)
09:00 – 10:00	**Physical Properties and Characterisation of Liquid Crystals** *Mamatha Nagaraj, University of Leeds*
10:00 – 11:00	**Liquid Crystal Devices: Past, Present, and Future** *Stephen M. Morris, University of Oxford*
11:00 – 11:30	Tea / Coffee Break
11:30 – 12:30	**Applied Modelling of Liquid Crystals** Nigel Mottram, University of Glasgow
12:30 - 13:00	**ZBD LCD Technology** *Guy Bryan-Brown, New Vision Display Ltd*

	The 2025 BLCS Annual Meeting
12:30 – 13:45	Registration (Continued) and Lunch
13:45 – 14:00	Opening Remarks – II
	Theory and Simulations of Liquid Crystals I *Chaired by Dr Dwaipayan Chakrabarti*
14:00 – 15:00	**The 2025 Ben Sturgeon Lecture** **Simulating Liquid Crystals: A Story of Structure, Motion, and Discovery** *Mark R. Wilson, Durham University*
15:00 – 15:20	**Spontaneous Oscillations in Heterogeneous Active Nematics** *Alexander Houston, University of Glasgow*
15:20 – 15:40	**Dipole-dipole interactions and the ferro-electric nematic phase: a simple model** *Andrew Masters, University of Manchester*
15:40 – 16:00	Sponsors Talks **Liquid crystals publications from Taylor & Francis** Nigel Balmforth, Taylor & Francis Group Ltd. **Reactive Mesogens for Virtual Reality** Stephen Fenner, Merck
16:00 – 16:30	Tea / Coffee Break

	Properties and Applications of Liquid Crystals I *Chaired by Dr Mamatha Nagaraj*
16:30 – 16:50	**Neutron scattering as a mesoscale probe for buried liquid crystals** *Oleksandr Tomchuk, ISIS Neutron and Muon Source*
16:50 - 17:10	**Bent-core liquid crystals as candidates for energy applications** *Alfonso Martinez-Felipe, University of Aberdeen*
17:10 - 17:30	**The Effect of Structural Modifications on the Stability Ferroelectric Nematic Phase** *Ewan Cruickshank, University of Aberdeen*
17:30 - 18:00	Tribute to Corrie Imrie
18:00 - 19:15	**Poster Presentations**

Day 3: Wednesday 9 April, Lloyd Suite (Hornton Grange)

	Liquid Crystals for Novel Materials *Chaired by Dr Rebecca Walker*
09:00 - 10:00	**The 2025 Gray Medal Lecture** **Design and Investigation of Nematic Systems** *Georg H. Mehl, University of Hull*
10:00 - 10:20	**Using Lateral Fluorination to Control the Formation of Ferroelectric Nematic and Smectic Phases** *Grant J. Strachan, University of Warsaw*
10:20 - 10:40	**Semi-soft elasticity and auxeticity in liquid crystal elastomers – how to get your material to do what you want!** *Thomas Raistrick, University of Leeds*
10:40 - 11:10	**Young Scientist Talk: From the twist-bend to polar order: exploring the rich chemistry of nematic and smectic liquid crystals** *Calum J. Gibb, University of Leeds*

11:10 - 11:30	Tea / Coffee Break
	Chiral Liquid Crystals *Chaired by Prof. Mark R. Wilson*
11:30 - 12:15	**Invited Talk** **Cellulose-based Liquid Crystalline Twisted Structures** *Maria Helena Godinho, NOVA University Lisbon*
12:15 - 12:35	**Bending and twisting in the hierarchical self-assembly of monodisperse mesogenic oligomers** *Chun Lam Clement Chan, University of Groningen and Princeton University*
12:35 - 12:55	**Pseudo Ferri-electric Switching in Spontaneously Chiral Liquid Crystals** *Jordan R. Hobbs, University of Leeds*
12:55 - 14:00	Lunch
	Topology in Liquid Crystals [Supported by the Royal Society of Edinburgh (RSE)] *Chaired by Prof. Stephen M. Morris*
14:00 - 15:00	**The 2024 Gray Medal Lecture** **Knotty Links Between Chiral Liquid Crystals, Particle Physics and Cosmology** *Ivan I. Smalyukh, University of Colorado Boulder and Hiroshima University*
15:00 - 15:20	**Transformations and Interactions of Point defects on a String of Half-Skyrmion** *Wentao Tang, Hong Kong University of Science and Technology*
15:20 - 15:40	**Temperature Reconfigurable Skyrmionic Solitons in Cholesteric Liquid Crystals** *Maryam Qaiser, University of Manchester*

15:40 - 16:00	**Liquid crystal skyrmions in external flows: from stretching to “skyrmion Hall effect”** *Mykola Tasinkevych, Nottingham Trent University*
16:00 - 16:30	Tea / Coffee Break
	Theory and Simulations of Liquid Crystals II *Chaired by Prof. Nigel Mottram*
16:30 - 16:50	**Spontaneous Chiral Symmetry Breaking in Polydisperse Achiral Near-Rigid Rods** *William S. Fall, Universite Paris-Saclay*
16:50 - 17:10	**Homogenised free energies for nano-doped cholesteric systems** *Prabakaran Rajamanickam, University of Strathclyde*
17:10 - 17:30	**All-atom simulations of CB6OIBeOn: a progress report** *Guinan Zhao, University of Manchester*
17:30 - 18:30	BLCS Annual General Meeting

Day 4: Thursday 10 April, Lloyd Suite (Hornton Grange)

	Liquid Crystal Devices *Chaired by Prof. Helen Gleeson*
09:15 - 10:00	**Invited Talk** **Laser-inscribed Liquid Crystal Photonics Elements** *Stephen M. Morris, University of Oxford*
10:00 - 10:20	**Photonic eigenmodes of 2D cylindrical cholesteric liquid crystal resonators** *Urban Mur, University of Ljubljana*
10:20 - 10:40	**Large area modelling of pixellated Liquid Crystal Displays** *Abhishek Ghosh, University of Glasgow*
10:40 - 11:00	**Liquid Crystal Diffraction Grating for Beam Steering Technology** *Qihao Han, University of Oxford*
11:00 - 11:30	Tea / Coffee Break
	Properties and Applications of Liquid Crystals II *Chaired by Prof. Georg H. Mehl*
11:30 - 12:15	**Invited Talk** **Photo-physical properties of liquid crystals; influence of molecular structure, shape and aggregation** *Mamatha Nagaraj, University of Leeds*
12:15 - 12:35	**Liquid Crystals with Non-Homeotropic Air Interface Anchoring Confined in Millimetre Sized Rectangular Surfaces** *Abigail Bond, University of Leeds*
12:35 - 12:55	**Thermochromic Liquid Crystal Sensors for Ultrasound Visualisation Applications** *Martha Turvey, University of Warwick*
12:55 - 14:00	Lunch
14:00 - 15:00	BLCS Committee Meeting

List of Posters: Tuesday 8 April (18:00 – 19:30)

Poster No.	Presenter	Organisation	Title
P1	Omar Aljohani	University of Manchester	Optical Effects of Monosaccharides and Disaccharides on the Tunability of Cellulose Nanocrystal (CNC) Photonic Films
P2	Ahlam Almamari	University of Strathclyde	The Flexoelectric Instability in Nematic Liquid Crystals
P3	Saud Al-Qabandi	University of Manchester	Towards the theory and simulation of the ferroelectric nematic phase
P4	Mona Alsubaie	University of Manchester	Micro-Rod Particle Dynamics in the Nematic Phase of Liquid Crystals Under Electric Fields
P5	Xi Chen	University of Birmingham	Understanding the Charge Transport Properties of Low-Symmetry Discotic Molecules
P6	Sarangi Krishna	Sheffield Hallam University	Simulations of liquid crystal tactoids and elastomers
P7	Oana Niculescu	University of Cambridge	Design and characterisation of Blue Phase Adaptive Optics correctors
P8	Charles Parton-Barr	University of Leeds	Deep Learning Driven Design of Novel Ferroelectric Nematic Liquid Crystals
P9	A. Pearson	University of Aberdeen	The Twist-Bend Smectic Phases: On the Role of Lateral Substituents
P10	Shona J. Ramsay	University of Aberdeen	Synthesis and Characterisation of Highly Fluorinated Ferroelectric Nematogen

Key	Topic
🟦	Workshop Lectures
🟧	Theory and Simulations of Liquid Crystals
🟨	Properties and Applications of Liquid Crystals
🟥	Liquid Crystals for Novel Materials
🟩	Chiral Liquid Crystals
🟫	Topology in Liquid Crystals
🟦	Liquid Crystal Devices
🟪	Posters

The Ben Sturgeon Lecture

Simulating Liquid Crystals: A Story of Structure, Motion, and Discovery

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From the early days of the liquid crystal display revolution, it was clear that liquid crystalline compounds posed a unique challenge. Synthetic chemists worked hard to unravel the link between bulk phase behavior and molecular structure, soon realizing that even minor molecular modifications could lead to dramatic shifts—not just in transition temperatures, but also in phase sequences. To many, these changes seemed almost mystical, defying simple logic.

Only later did researchers recognize the underlying reason: liquid crystal phases exist in a delicate free-energy landscape, where small stability differences separate multiple possible structures. Subtle variations in molecular packing or local interactions can be enough to stabilize new phases or disrupt dominant ones, revealing previously unseen behaviour. This understanding paved the way for recent discoveries, including the ferroelectric nematic, antiferroelectric nematic, twist-bend nematic, polar-twisted nematic, and heliconical ferroelectric nematic phases, alongside new smectic structures.

Molecular simulations have played a crucial role in deciphering liquid crystal phase formation, offering molecular-level insights into how functional groups and conformational changes influence phase behaviour. Early simulations were constrained by limited computational power and by the sophistication of models. However, recent advancements in both have driven significant breakthroughs.

This talk provides some historical perspective into the development of computer simulations of liquid crystals, providing insight into the intricate interplay of structure and molecular motion in these phases through coarse-grained and atomistic molecular modelling. Results will be presented[1–5] shedding light on the molecular organization in the nematic-twist bend phase, the ferroelectric nematic phase, columnar phases and lyotropic self-assembled structures.

1 G. Yu and M. R. Wilson, All-atom simulations of bent liquid crystal dimers: the twist-bend nematic phase and insights into conformational chirality, *Soft Matter*, 2022, **18**, 3087–3096.
2 M. R. Wilson and G. Yu, Computer Simulations of a Twist Bend Nematic (NTB): A Coarse-Grained Simulation of the Phase Behaviour of the Liquid Crystal Dimer CB7CB, *Crystals*, 2023, **13**, 502.
3 M. R. Wilson, G. Yu, T. D. Potter, M. Walker, S. J. Gray, J. Li and N. J. Boyd, Molecular Simulation Approaches to the Study of Thermotropic and Lyotropic Liquid Crystals, *Crystals*, 2022, **12**, 685.
4 G. Yu, M. Walker and M. R. Wilson, Atomistic simulation studies of ionic cyanine dyes: self-assembly and aggregate formation in aqueous solution, *Physical Chemistry Chemical Physics*, 2021, **23**, 6408–6421.
5 F. Chami and M. R. Wilson, Molecular Order in a Chromonic Liquid Crystal: A Molecular Simulation Study of the Anionic Azo Dye Sunset Yellow, *Journal of the American Chemical Society*, 2010, **132**, 7794–7802.

The 2024 Gray Medal Lecture

Knotty Links Between Chiral Liquid Crystals, Particle Physics and Cosmology

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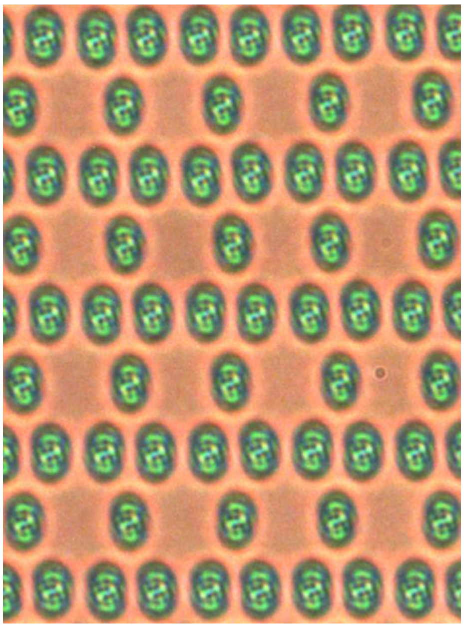
Feynman's words “What I cannot create, I do not understand” inspire us to use the power of topology and chirality to experimentally re-produce phenomena and "bring to life" theories from diverse fields like particle physics and cosmology. Even physically-sound models that turned out not describing the real World around us can materialize in the artificial "meta-World" table-top experiments that we meticulously design. I will first discuss how vortex knots in chiral liquid crystals can exhibit atom-like behavior, including fusion, fission and self-assembly into various crystals (one example shown on a polarizing optical micrograph to the right) with giant electrostriction properties. These findings will let us admire the beautiful history of the early model of atoms by Lord Kelvin, and the origins of mathematical knot theory, as well as the very last poem by Maxwell related to them. I will discuss how the chiral liquid crystalline topological solitons, nonsingular vortex knots and multi-component links relate to the modern-day topological models of subatomic particles. Finally, I will show that the vortices (nonsingular disclinations) in chiral liquid crystals interact with light similar to what was predicted for the elusive cosmic strings, with knots and crystalline arrays of vortices allowing to spatially localize beams of light into closed loops and knots.



The 2025 Gray Medal Lecture

Design and Investigations of Nematic Systems

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The investigation of thermotropic nematic molecules and the synthesis of new systems has remained at the forefront of LC research over many years. This is due to the technological relevance of the nematic phase and is also linked to the importance of advancing molecular design rules in fundamental research. Collaborative research has been stimulated by responding to theoretical predications of a number of nematic related phases, such as the biaxial nematic (Nb), the twist bend nematic (Ntb) and more recently the ferroelectric nematic (Nf), to name just a few of the nematic subphases. These investigations require a range of molecular architectures, ranging from small molecules, to dimers, oligomers and to dendrimers and LC nanoparticle systems. For several nematic subphases spontaneous deracemization and the formation of chiral assembly structures has been observed. This is often difficult to identify when the chiral structures and the associated helicity as well as chiral domain sizes are far below the visible wavelength range. The challenges to identify and measure LC properties, including helix formation over a range of molecular architectures will be presented, making use of the results of a number of methods, including XRD and circular dichroism techniques. In this context iterative design progression for the optimisation of molecular architectures will be discussed and set in context of related work.

Cellulose-based Liquid Crystalline Twisted Structures

Maria Helena Godinho
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Twisted structures are widespread in nature, with cellulose serving as the structural backbone of various helical systems across molecular, nano, micro, and macro scales. These helicoidal arrangements contribute to structural coloration, enhanced mechanical properties, and motion. This presentation explores cellulose-based liquid crystalline chiral molecular systems, nanoscale helicoidal structures, cellulose nanocrystals, water interactions, and out-of-equilibrium colorful structures formed by cellulose derivatives. It then examines micro- and millimeter-scale examples, such as helical formations in vascular leaf petioles, tendrils, and Erodium fruit awns, highlighting their role in adaptive shape changes and movement. The findings suggest a need for further research on out-of-equilibrium liquid crystalline systems and bio-inspired twisted functional materials, offering a comprehensive overview of the current understanding and future potential of these natural helicoidal structures.

Acknowledgements
The author acknowledge to INPACTUS, FCT-Fundação para a Ciência e a Tecnologia, I.P., in projects LA/P/0037/2020, UIDP/50025/2020, UIDB/50025/2020, of the Associate Laboratory Institute i3N and 2022.04191.PTDC.

R.R. da Rosa, S.N. Fernandes, M. Mitov, M.H. Godinho, *Advanced Functional Materials*, 2024, **34**(35), 2304286.

Laser-inscribed Liquid Crystal Photonics Elements

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In this presentation, I will describe our work on using two-photon direct laser writing to fabricate new optical elements in polymerisable nematic liquid crystals and liquid crystal conjugated polymers. These photonics elements include switchable diffraction gratings, computer generated holograms, tunable optical vortex beam generators, optical aberration correctors, switchable Fresnel Zone Plates, and tunable waveguides (see **Figure 1** for examples). We demonstrate how multiple optical elements can be embedded into a single liquid crystal device, requiring only a pair of electrodes to active the elements, thereby negating the need for the complex electrode architecture found in conventional spatial light modulators. By varying the applied voltage, we also show how these devices can be tailored to function at any desired wavelength, a feature that is not readily achievable for static diffractive optic elements. We conclude by demonstrating how the technique can be combined with photoalignment layers to enable high quality spatial patterning of liquid crystal conjugated polymers.

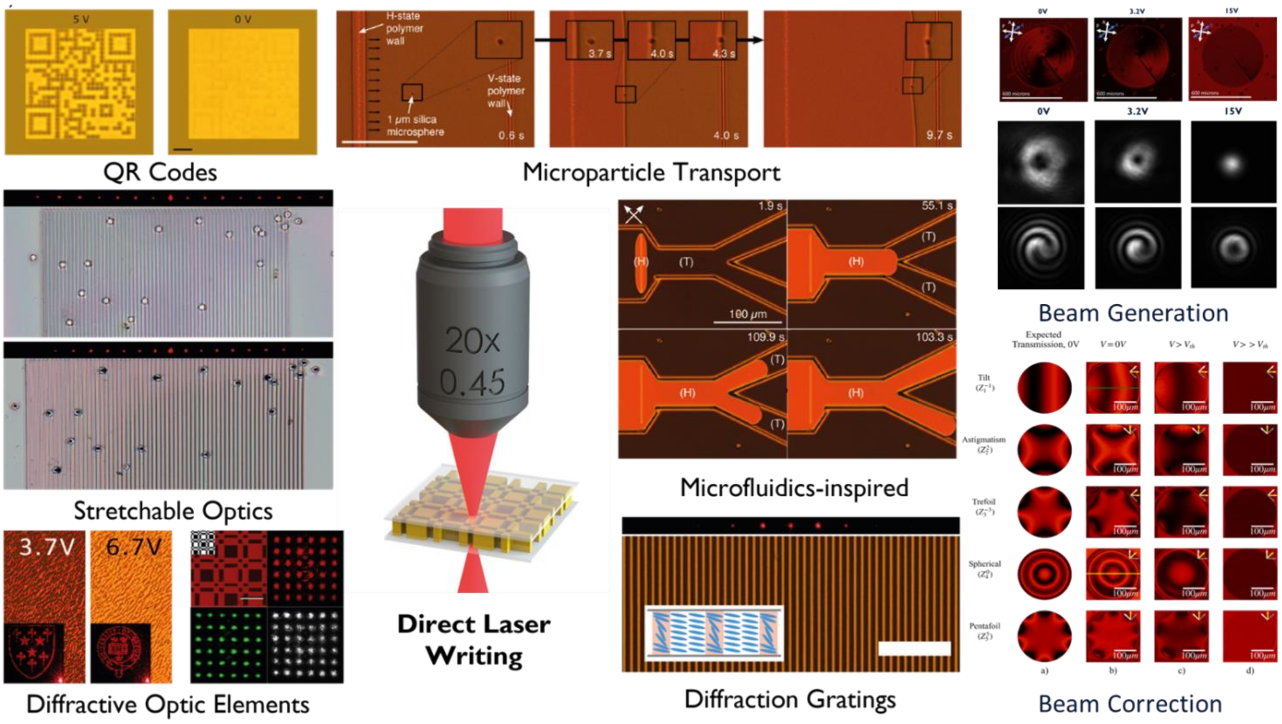

Figure 1. Liquid crystal optical elements fabricated using two-photon direct laser writing.

Photo-physical properties of liquid crystals; influence of molecular structure, shape and aggregation

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Fluorescence in liquid crystals (LCs) is highly desirable for applications in opto-electronics, photo-voltaics and light emitting diodes [1]. Similar to many other fluorescent materials, excimer formation and emission is an interesting and useful phenomena in liquid crystals too. Applications and technologies have been developed from both using and quenching such effects. However fluorescence properties of LCs are often investigated only in dilute solutions and in geometries such as cuvettes due to complex experimental difficulties [2]. Whilst LCs can be highly fluorescent in solution, once they are concentrated, in a neat form, in a device, their fluorescence behaviour including emission and quenching properties [3] change and cannot be directly correlated to the results from dilute solutions.

In this presentation, intrinsic fluorescence properties of liquid crystals measured in neat LCs in sandwich devices, will be presented. The effect of molecular shape and chemical structure of the LC and the inherent symmetry of the phase on their photo-physical properties will be discussed. Specifically, the influence of molecular pair formation on the emission properties and the monomer and excimer formation, in different device geometries, will be discussed. Mechanisms of fluorescence quenching and time dependent studies of aggregation and crystallisation induced emission enhancement will be shown.

References

1. M. Klock W. Rettig J. Hofkens, M. vanDamme, F. C. De Schryver, J. Photochem Photobio A, 1995, **85**, 11.
2. J. Hobbs, J. Mattsson, M. Nagaraj, *Crystals*, 2024, **14**, 362.
3. J. Mei, N. L. C. Leung, R. T. K. Kwok, J. W. Y. Lam, and B. Z. Tang, Chem. Rev., 2015, **115**, 11718.

The 2025 BLCS Young Scientist Talk

From the twist-bend to polar order: exploring the rich chemistry of nematic and smectic liquid crystals

Calum J. Gibb[1], Jordan Hobbs[2], and Richard J Mandle[1,2]
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Ferroelectric nematic (N_F) liquid crystals combine liquid-like fluidity and orientational order of conventional nematics with macroscopic electric polarization comparable in magnitude to solid state ferroelectric materials [1-5]. Here, we present a systematic study of twenty-seven homologous materials with various fluorination patterns, giving new insight into the molecular origins of spontaneous polar ordering in fluid ferroelectric nematics. Beyond our initial expectations, we find the highest stability of the N_F phase to be in materials with specific fluorination patterns rather than the maximal fluorination which might be expected based on simple models (**Figure 1**). We find a delicate balance between polar and apolar nematics which is entirely dictated by the substitution of the fluorine atoms. Aided by electronic structure calculations, we show this to have its origins in the radial distribution of charge across the molecular surface, with molecules possessing a more oscillatory distribution of electrons across their surfaces possessing a higher propensity to form polar nematic phases. This work provides a new set of ground rules and designing principles which can inform the synthesis of future ferroelectric nematogens [6].

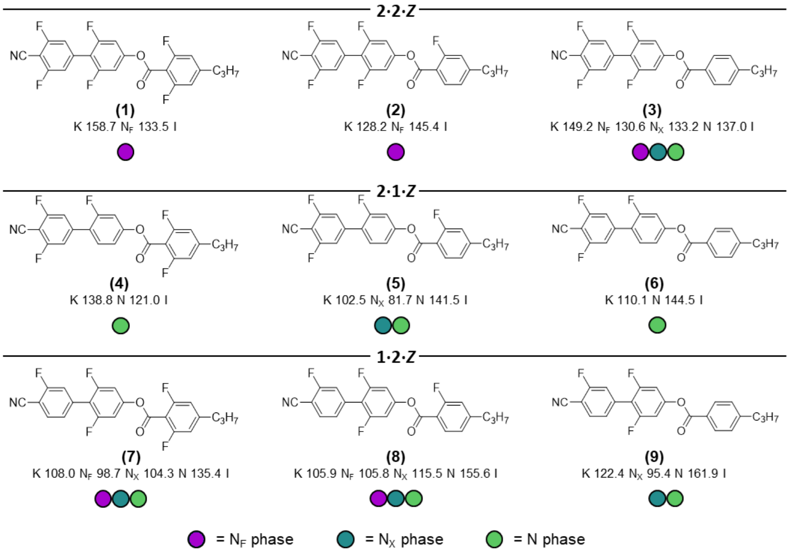

Figure 1. The chemical structures, phase sequences and associated transition temperatures (°C) of materials **1-9**. Of note, maximum fluorination does not result in the most stable N_F phase.

K = melting point; N_F = ferroelectric nematic; N_X = antiferroelectric nematic; N = nematic; I = isotropic liquid.

[1] R. J. Mandle, S. J. Cowling, J. W. Goodby, Phys. Chem. Chem. Phys., 2017,**19**, 11429.; [2] H. Nishikawa, K. Shiroshita, H. Higuchi, Y. Okumura, Y. Haseba, S. I. Yamamoto, K. Sago, and H. Kikuchi, Adv. Mater., 2017 29, 1702354.; [3] N. Sebastián, L. Cmok, R. J. Mandle, M. R. De La Fuente, I. Drevenšek Olenik, M. Čopič, and A. Mertelj, l, Phys. Rev. Lett. 2020, 124, 037801.; [4] X. Chen, E. Korblova, D. Dong, X. Wei, R. Shao, L. Radzihovsky, M.A. Glaser, J.E. Maclennan, D. Bedrov, D.M. Walba, N.A. Clark, Proc. Natl. Acad. Sci. U.S.A., 2020 117, 14021.; [5] R. J. Mandle, N. Sebastián, J. Martinez-Perdiguero, and A. Mertelj, Nat. Commun., 2021, 12, 4962.; [6] C. J. Gibb, J. Hobbs, and R. J. Mandle, J. Am. Chem. Soc., 2025. DOI: 10.1021/jacs.4c16555.

Contributed Talks

Liquid Crystals with Non-Homeotropic Air Interface Anchoring Confined in Millimetre-Sized Rectangular Surfaces

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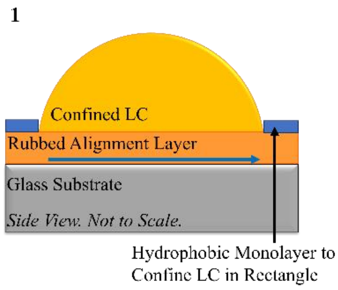
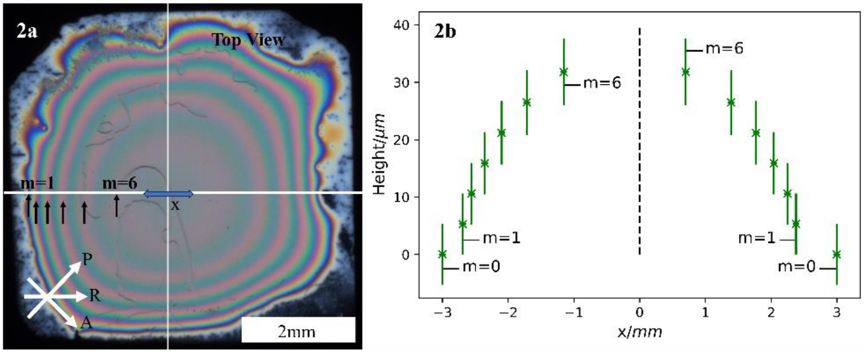
This talk extends on work by Bond *et al.*[1], where E7 nematic liquid crystal (LC) 'semi-droplets' were confined into chemically patterned rectangles of widths : lengths of 6-13mm : 6-20mm, with rubbed planar-to-homeotropic anchoring from the substrate to air/LC interfaces. This range extended upon recent literature, as it is expected that the large sizes will make LC-based sensors more sensitive and be easier to read without a microscope. The height of the semi-droplets was measured using the full-wave condition with polarised light imaging (Figure 2). A simple, non-LC specific geometric height variation model was derived and compared to a model for a similar system by Cousins *et al.*[2]. Cousins *et al.*'s work was extended by experimental validation over the entire width, as the models agreed well with measurement for maximum height $\lesssim$ 50μm, even with the ratio of width : capillary length > 1. This implies minimal gravitational effects on their shape below this height.
To extend the work by Bond *et al.*[1] LCs that are expected to have non-homeotropic anchoring at the air/LC interface, e.g. MLCs 2081 and 7023[3], are confined in these rectangular shapes. As analytes can promote planar or homeotropic alignment, and most LC-based sensing relies on the change in director field under polarised imaging, it is important to understand both homeotropic and planar air/LC interfaces within these systems. MLC 2081 and E7 have surface tensions of $\sim 0.024 \mathrm{Nm}^{-1}$ whereas MLC 7023 has a 'low'[3] value, therefore is particularly interesting for it's width : capillary length ratio.



1: *Diagram of chemically patterned glass to confine LC in rectangles with rubbed planar substrate to homeotropic air/LC interface anchoring.*



2. *Measurement of semi-droplet height:* a: *Example sample of confined E7 between crossed polarisers,* b: *Corresponding spacing of pink birefringent fringes, m, and their related heights, along horizontal white line on 2a. The vertical white line is the analysis along the length of the sample, as can be seen in Bond* et al.[1]

References
[1] A. Bond, T. Moorhouse, S.A. Peyman, H.F. Gleeson. 2025. ***Paper under review in Liquid Crystals.*** *Figures slightly adapted from paper.*
[2] J.R.L. Cousins, *et al. Physical Review E.* 2023. **107**, p.034702.
[3] D.A. Paterson, *et al. Langmuir.* 2020. **36**, p.6436-6446.

Bending and twisting in the hierarchical self-assembly of monodisperse mesogenic oligomers

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The design of mesogenic oligomers offers an exceptional opportunity to tailor intermolecular interactions and supramolecular assembly by controlling both local mesogen geometry and oligomer chain conformation. These parameters can be tuned by changing the length and sequence of the oligomer. To probe the effect of oligomer length and sequence, we developed a new synthetic strategy based on iterative exponential growth synthesis to yield monodisperse sequence-defined oligomers. By preparing homooligomers ranging from dimer to octamer, we demonstrate that the self-assembled crystalline phase displays different types of curvature (Gaussian or cylindrical) and the curvature exhibited depends critically on the oligomer length, which range from dimer to octamer. Length-dependent thermodynamic and kinetic effects tune the degree of crystalline order in these oligomers, which then drive the formation of scrolled sheets in shorter oligomers and twisted ribbons in longer oligomers. Subsequently, through analyzing the phase behavior of two asymmetric heterodimers that differ only in mesogen sequence, the effects of oligomer sequence can be examined. While both heterodimers crystallize into scrolled nanocylinders, their higher order supramolecular assemblies and associated optical properties differ drastically. Nanocylinders of one dimer twist into bundles and exhibit bulk optical activity while in the other dimer, the nanocylinders arrange into a spiral arrangement, which do not appear chiral optically. These studies highlight how oligomer length and sequence interplay with mesogen geometry and crystalline packing to drive multi-scale self-assembly into spontaneously chiral assemblies that could be exploited as tunable chiroptical devices.

The Effect of Structural Modifications on the Stability Ferroelectric Nematic Phase

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The ferroelectric nematic phase, N_F, has become one of the key research topics in the field of liquid crystal research since its experimental discovery in 2017[1,2] and assignment in 2020[3], with an ever growing library of compounds and a wide range of potential applications being identified.[4–6] The N_F phase is a variant of the conventional nematic phase, N, which is the least ordered liquid crystalline phase. To date there have been around a 150 low molar mass compounds which exhibit the phase[7] and the vast majority of these can be described using the three following structures, namely RM734[1], DIO[2] and UUQU-4N[8], Figure 1. Here we report the transitional properties of a variety of new three ring compounds with a range of structural modifications which are based on the compound RM734 and exhibit the ferroelectric nematic phase.

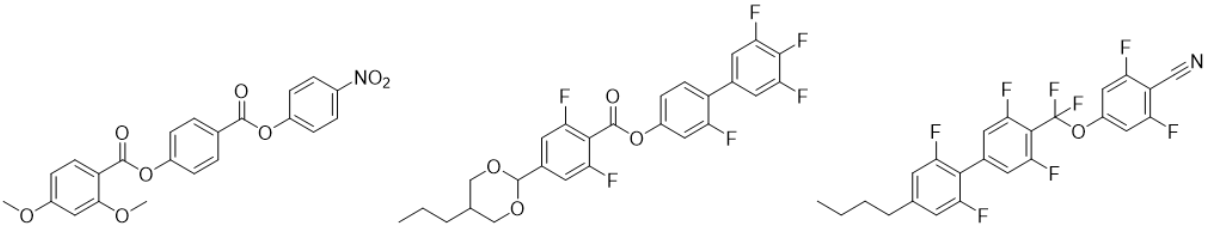

Figure 1. Molecular structure of (left) RM734, (middle) DIO and (right) UUQU-4N.

[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] Li, J. *et al*. *Giant*, **11**, 100109, (2022).

[5] Nacke, P. *et al*. *Scientific Reports*. **14**, 4473 (2024)

[6] Strachan, G. *et al*. *J. Am. Chem. Soc.* **147**, 6058–6066 (2025)

[7] Cruickshank, E. *ChemPlusChem.* e202300726 (2024).

[8] Manabe, A. *et al*. *Liq. Cryst.* **48**, 1079-1086, (2021).

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Spontaneous Chiral Symmetry Breaking in Polydisperse Achiral Near-Rigid Rods

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Understanding the transfer of chirality from the molecular to the macroscopic scale poses a significant challenge in soft and biological condensed matter physics. Many nanorods of biological origin not only have chiral molecular features but also exhibit a spread in contour length leading to considerable size dispersity [1]. On top if this, conformational fluctuations along the rod backbone are ubiquitous but their role in chirality transfer remains difficult to entangle from that of their native chirality imparted by the rod shape or surface architecture [2]. We report spontaneous entropy-driven chiral symmetry breaking from molecular simulations of nematic liquid-crystals formed from achiral hard cylinders with marginal backbone flexibility and a continuous spread in length [3]. The symmetry-breaking is caused by long-lived chiral conformations of long rods residing in the tail of the rod length distributions leading to non-zero residual chirality within the nematic system. Using a simple phenomenological theory to rationalize the simulations we demonstrate that a combination of contour length polydispersity and weak unbiased conformational fluctuations of achiral rods can drive spontaneous chiral symmetry breaking at the macroscale at medium length polydispersity.

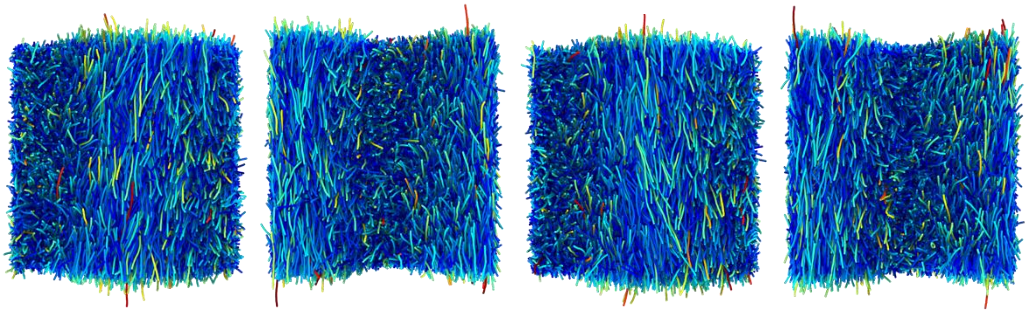

Figure 1. Snapshots of the twisted Cholesteric phase formed by polydisperse achiral near rigid-rods. Rods are coloured using a rainbow colour scheme according to their length.

[1] H. H. Wensink, *Crystals,* 2019, **9(3)**, 143.
[2] M. M. C, Tortora, G. Mishra, D. Prešern and J. P. K. Doye. 2020, Science Advances **6(31)** eaaw8331.
[3] W. S. Fall and H. H. Wensink. *Unpublished,* 2025.

Large area modelling of pixellated Liquid Crystal Displays

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We present a modelling framework for Liquid Crystal Displays that allows fast simulation of large areas of pixelated displays. This dynamic model considers the orientation of the director (in either director angle or Q-tensor descriptions) and the electric potential, integrating elastic, weak anchoring, dielectric and flexoelectric effects. Through approximations to the director and electric potential dependence on the coordinate perpendicular to the display substrates, the three-dimensional behaviour of the system is reduced to a two-dimensional model that retains the ability to accurately model pixel edge effects and fringe fields. Computational simulations in COMSOL Multiphysics allow a comparison of this two-dimensional approximation to a full three-dimensional model, showing the simpler, faster model accurately predicts director reorientation under applied fields. The speed of the two-dimensional model (over 50 times faster than the three-dimensional model) allows greater understanding of non-periodic patterns of on and off pixels and provides an efficient tool for optimising electro-optical performance. An example is provided in the Figure below, where a 324-pixel system (pixel electrode dimension = 5 microns, inter-electrode gap = 0.5 microns) simulated for 5 seconds of modelled time, was completed within 30 minutes of computational time.

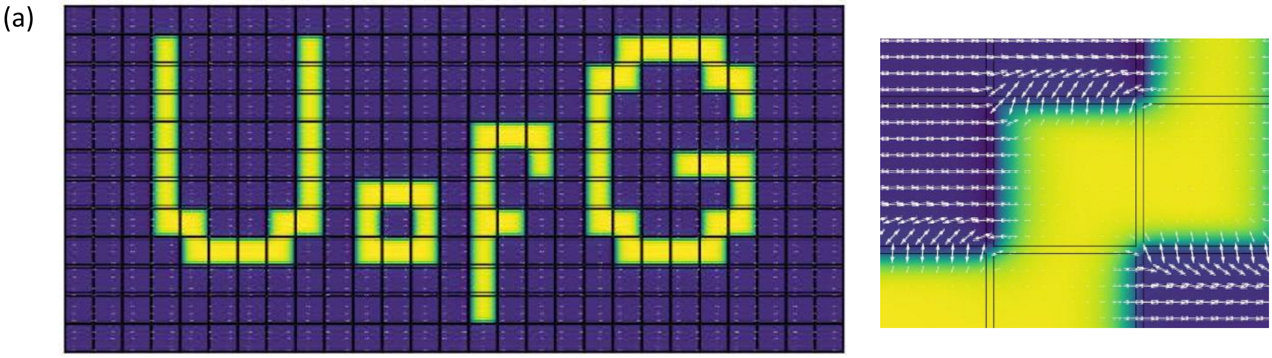

Figure: (a) example of a large-area, 324 pixel simulation. Pixels forming the “UofG” shape are switched on and colour indicates the average director tilt angle (yellow = homeotropic, blue = planar) (b) enlarged area of (a) showing the average director orientation (white double-arrows).

Liquid Crystal Diffraction Grating for Beam Steering Technology

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Beam steering is a crucial technology for applications such as visible light communication, LiDAR, and AR/VR displays. This study investigates three liquid crystal (LC)-based diffraction grating approaches to achieve rapid response, low power consumption, a wide diffraction angle, and highly tunable beam steering.

First, a flexoelectric diffraction grating is developed using the bent-core LC dimer CB7CB. The strong flexoelectric response enables real-time voltage-controlled periodic bend-splay structures, offering precise control over the far-field diffraction pattern. An advanced novel nonlinear model is proposed to more accurately describe the grating's behavior, outperforming previous linear models. Experimental validation demonstrates rapid response, low applied voltage, and a second-order diffraction angle of 35°.
Second, a cholesteric liquid crystal (CLC) switchable and rotatable diffraction grating is achieved in a homotropic cell with a stabilized Uniform Lying Helix (ULH) state. The introduction of a small amount of CB7CB enhances asymmetry in the flexoelectro-optic tilt angle. When driven by a specially tailored waveform, this induces torque on the helix axis, enabling electrically controlled 360-degree in-plane rotation of the helix axis (as shown in Figure 1), which in turn causes the far-field diffraction pattern to rotate accordingly.

Third, a polarization grating-based beam steering system is demonstrated for fast-response, multi-location holographic display applications. By integrating circularly polarized laser emission with tunable nematic phase shifters and fixed polarization gratings, the system achieves discrete multi-location beam steering. Together, these approaches provide promising solutions for next-generation dynamic beam-steering devices.

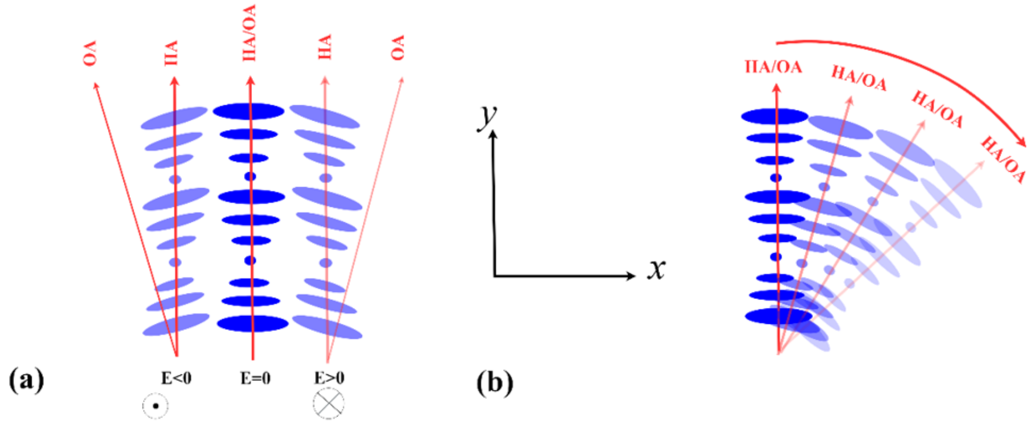

Figure 1. (a) Illustration of the optic axis (OA) rotation in a CLC under an electric field applied perpendicular to the helix axis (HA). (b) An example of a rotation of the helix axis (HA)/optic axis (OA) in a CLC.

Pseudo Ferri-electric Switching in Spontaneously Chiral Liquid Crystals

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Spontaneous chiral symmetry breaking is a phenomena observed in some of the most exciting areas of modern liquid crystal science. The recent observation of spontaneous heliconic formation of degenerate handedness in polar nematic and smectic liquid crystals [1,2] is reminiscent of the exotic spin textures of ferro-magnetic systems, normally difficult to form in ferroelectric systems due to lattice strain effects but allowed here due to the fluidity of the system.

In this talk some of the properties of this new phase will be presented including pseudo ferri-electric switching and tilt removal. Evidence that helix formation can be either a 1st order or 2nd order phase transition type will be presented [3] as well as a demonstration of how phase ordering can affect the morphology of the phase.

[1] C. J. Gibb, *et al. Nat Commun* **15**, 5845 (2024)
[2] J. Karcz *et al. Science* **384**,1096 (2024)
[3] J. Hobbs et. al. arXiv:2502.08551 [cond-mat.soft] (2024)

Spontaneous oscillations in heterogeneous active nematics

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The framework of active nematics may be used to model many living systems, including cell layers and bacteria.[1] The study of active nematics has focused on uniform activity, but real biological systems are not homogeneous, rather they have population variance or are composed of different species. 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 living systems and to enable desired dynamics to be engineered in active matter.

A central feature of active nematics is that, when confined, they exhibit a transition to a flowing state, provided their activity exceeds a critical value.[3] In this context we show that activity variation allows control of the structure of the flowing state and, most strikingly, can lead to oscillatory dynamics. We show analytically that the behaviour of the confined active nematic can be mapped onto a dynamical system, the coefficients of which are determined by the activity variation, and confirm these results numerically. We find that an activity gradient can induce oscillations, and in this case determine how the properties of the system influence the oscillation frequency.

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

Bent-core liquid crystals as candidates for energy applications

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Liquid crystals form multiscale nanostructures that respond to external stimuli, with the potential to yield several functionalities.[1] They can create controlled 1D (columnar), 2D (smectic), and 3D (bicontinuous) channels that promote transport of ions or charges, with application in electrochemical devices, such as, fuel cells, solar cells, batteries, among others.[2] Bent-core liquid crystals (BCLCs) are characterised by their non-linear, bent-shaped molecular structures, in contrast to conventional rod-like liquid crystals. BCLCs' archetypical structure involves several aromatic rings forming an angle through a central meta-substituted ring, containing various linking groups and flexible terminal chains at one or both ends, which reduce the melting point. BCLCs can exhibit spontaneous polarization and chirality even in the absence of chiral centers within the molecules, resulting in antiferroelectric and ferroelectric behaviour that can be useful for various technological applications, including non-linear optics and energy storage.[3] In this talk, I will present some of our recent work to develop functional BCLCs as electrolyte candidates in energy devices. More specifically, I plan to focus on our results obtained for ethylenoxide-decorated mesogens labelled as **TEG-n-Bx-14**, and their complexes with various ionic salts (triflate and bistriflate) containing lithium and sodium as countercations, see Figure 1. I will describe their synthetic routes, summarise their physic-chemical characterisation through a combination of optical, spectroscopic, and computational techniques, and I will discuss their conductivity and ferroelectric behaviour. Furthermore, I will discuss how the presence of azobenzene groups (X ≡ N=N) introduces the exciting possibility to exert light control of their functionality, via trans-to-cis photoisomerization.[4]

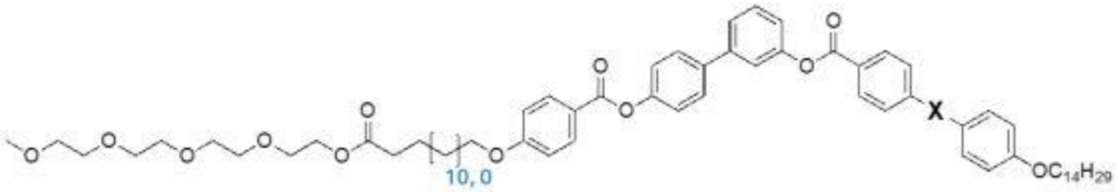

Figure 1. Chemical structure of the **TEG-n-Bx-14** series: n = 0, 10, X ≡ N=N (azobenzene), C=O (ester), or nil (biphenyl).

References

1. Martinez-Felipe, A., Liquid crystal polymers and ionomers for membrane applications. Liquid Crystals, 2011. **38**(11-12): p. 1607-1626.
2. Cho, B.K., Nanostructured organic electrolytes. RSC Advances, 2014. 4(1): p. 395-405.
3. Martinez-Felipe, A., et al., Bent-core liquid crystals joining the ethylene-oxide/lithium ion tandem: Ionic conductivity and dielectric response towards new electrolytes for energy applications. Journal of Molecular Liquids, 2023. **390**: p. 123100.
4. Liebsch, J., et al., Tailoring the dielectric and ferroelectric response of mixtures containing bent-core liquid crystals through light-irradiation and composition. JOURNAL OF MOLECULAR LIQUIDS, 2024. **399**: p. 124371-124371.

Dipole-dipole interactions and the ferro-electric nematic phase: a simple model

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In 1916, Born[1] proposed that dipole-dipole coupling provided the driving force for ferro-electric nematic (N_F) formation. In the following years, however, theoreticians advanced precisely the opposite view, arguing that dipole-dipole interactions destabilised the N_F phase[2]. Recently, Osipov[3] showed that boundary effects could affect the properties of an N_F phase and possibly its very existence.

Atomistic simulations generally use the Particle Mesh Ewald sum technique to treat dipole-dipole interactions, but boundary conditions come into play here also[4]. Conducting, or “tin foil”, boundary conditions are standardly used, but to our knowledge the effects of using other boundary conditions, such as an insulating boundary, have not been studied.

To study the effect of boundary conditions on the stability of the N_F phase, we present simulation results for a classical Heisenberg spin lattice model[5] with additional dipole-dipole interactions. We will discuss how the nature of the N_F phase changes with strength of dipole moment, system size and boundary conditions. The simulation results will also be compared with the predictions of a simple mean-field theory.

[1] M. Born, *Kitzinger. Preuss. Akad Wiss*., 1916, **30**, 614.
[2] See, e.g.,A. G. Khachaturyan, *J. Phys. Chem. Solids*,1975, **36**, 1055.
[3] M. A. Osipov, *Liquid Crystals Reviews*, 2024, **12**, 14; *ibid*. *Liquid Crystals*, 2024, **51**, 2349.
[4] See, e.g., M. P. Allen and D. J. Tildesley, *Computer Simulation of Liquids*, Oxford University Press, 2017.
[5] For a recent study, see, e.g., C. Holm and W. Janke, Phys. Rev. B **48**, 936 (1993)

Photonic eigenmodes of 2D cylindrical cholesteric liquid crystal resonators

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In this study, we analyze the spectra and optical modes of 2D Cholesteric Liquid Crystal (CLC) resonators using the Finite Difference Frequency Domain (FDFD) method. Specifically, we examine two characteristic cross sections of a 3D CLC droplet with a typical radial spherical structure, both of which we approximated by analytical director fields. Our results demonstrate the presence of edge modes, defect modes, and Whispering Gallery Modes (WGMs) in cylindrical CLC layers, as well as the novel hybrid WGM-defect modes. We briefly discuss the influence of different parameters on these modes and compare the FDFD method with the Finite Difference Time Domain (FDTD) method. This work provides insights into understanding optical modes in 3D CLC droplets, essential for designing lasers and spherical reflectors.

Temperature Reconfigurable Skyrmionic Solitons in Cholesteric Liquid Crystals

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Solitons, self-sustained localized waves, are fundamental to many physical systems, from nonlinear optics to condensed matter physics. In liquid crystals, topological solitons such as torons exhibit remarkable stability and tunability, making them intriguing candidates for both fundamental studies and potential applications.

This talk will present recent investigations into torons in chiral nematic liquid crystals (CNLCs), particularly in the temperature-responsive material 4-[(S,S)-2,3-epoxyhexyloxy]-phenyl-4-(decyloxy)-benzoate (W46). A key feature of this system is the strong temperature dependence of its pitch, which enables a reversible transformation between torons and cholesteric fingers. Upon decreasing pitch, torons act as nucleation sites for cholesteric finger growth, while increasing the pitch leads to their retraction, reforming torons. Despite significant morphological deformations during heating–cooling cycles, torons remain topologically protected. Additionally, cooling rate variations influence toron density, with faster cooling leading to higher toron number density.

Further work explores the influence of external fields on toron stability and dynamics in the presence of cholesteric fingers, shedding light on new mechanisms for controlling solitonic structures in soft matter systems. These findings contribute to the broader understanding of topological solitons and their potential applications in optics, materials science, and beyond.

Semi-soft elasticity and auxeticity in liquid crystal elastomers – how to get your material to do what you want!

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Liquid crystal elastomers are lightly cross-linked elastomeric materials containing liquid crystal components. Under deformations perpendicular to the nematic director, LCEs have been reported to display one of two distinct behaviours: semi-soft elastic (SSE) or an auxetic response, previously (and erroneously) described as a mechanical Freedericksz transition. [1,2] Auxetics are materials displaying a negative Poisson's ratio – they get thicker when stretched.

In the soft elastic response, there is little-to-no elastic cost of deformation due to the continuous in-plane rotation of the director to align with strain. The 'semi' in 'SSE' comes from the initial 'high' modulus region observed in the stress-strain curve, followed by a plateau. [1] In the SSE response, the order parameter is constant and optical textures, called "stripe domains", form to minimise macroscopic shear. [1,3] Conversely, auxetic LCEs deform with a reduction in uniaxial order and an emergence of biaxial order. Auxeticity arises due to out-of-plane rotations of mesogenic units. [4] Additionally, the LCE remains optically clear throughout the deformation.

[2] The question still remains as to why certain LCEs deform via the SSE and others deform via an auxetic deformation. Here, a series of sidechain liquid crystal elastomers with varying crosslink density is studied. Higher crosslink density samples display a clear auxetic response. [5] At lower crosslink densities, the behaviour is consistent with the SSE response. At intermediate crosslink density, transitionary behaviour with similarities to both the auxetic and SSE response is observed. These results are described along with theoretical insight that suggests design rules for each.

[1] M. Warner, and E. M. Terentjev. *Liquid crystal elastomers.* OUP, 2013, Oxford.
[2] D. Mistry, *et al*. Coincident molecular auxeticity and negative order parameter in a liquid crystal elastomer. *Nature communications*, 2018, 9(1), 5095.
[3] M. Warner, and E. M. Terentjev. *Nematic elastomers—a new state of matter?*. Progress in Polymer Science, 1996, 21(5) 853-891.
[4] T. Raistrick, *et al.*, Understanding the physics of the auxetic response in a liquid crystal elastomer. *Physical Review Research*, 2021, 3(2), 023191.
[5] Z. Wang, *et al*. Direct observation of biaxial nematic order in auxetic liquid crystal elastomers. *Materials*, 2022, 16(1), 393.

Homogenised free energies for nano-doped cholesteric systems

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Colloidal nanoparticles, like quantum dots and gold nanoparticles, offer exciting possibilities for manipulating the optical and mechanical properties of liquid crystals when dispersed within them. This study investigates the impact of such nanoparticles on confined cholesteric systems using a homogenized Landau-de Gennes framework. We reveal the emergence of biaxial liquid crystal phases in spatially homogeneous systems, even when the colloidal particles themselves are uniaxial. Additionally, we explore the rich landscape of metastable states and their transitions in inhomogeneous systems, extending previous work that did not incorporate nanoparticles.

Using Lateral Fluorination to Control the Formation of Ferroelectric Nematic and Smectic Phases

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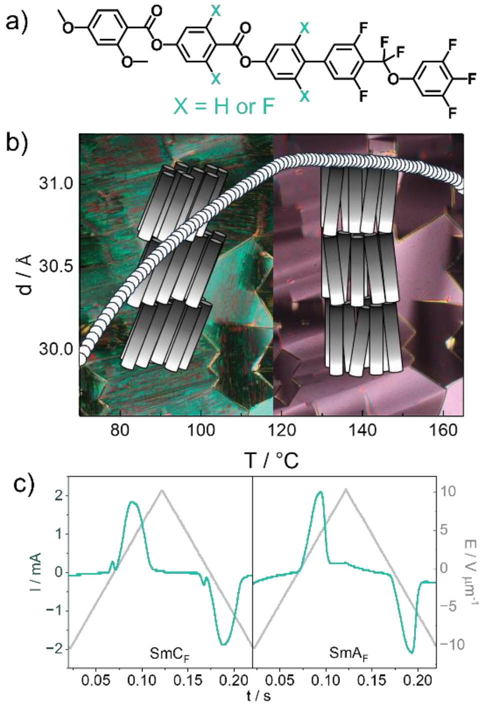

Figure 1 a) The structures of the molecules studied; b) POM textures of the SmC$_F$ and SmA$_F$ phases with (overlaid) the change in layer spacing on cooling and (inset) sketches of the phase structure; c) switching current generated in the SmC$_F$ and SmA$_F$ phases.

The 2017 discovery of the ferroelectric nematic (N$_F$) phase revealed an entirely new area of liquid crystals. Since then, a range of new polar phases have been discovered, including orthogonal and tilted ferroelectric smectic phases (SmA$_F$ and SmC$_F$).[1] However, reports of these new polar phases are limited, and the relationship between molecular structure and phase formation is not clear.

We recently reported a rare example of a mesogen forming a complete sequence of ferroelectric phases, N$_F$, SmA$_F$, and SmC$_F$.[2] Unusually for a smectic LC, this molecule contains no alkyl chains. This highlights the unusual relationship between molecular structure and the formation of these ferroelectric LC phases. Building on this observation, we investigated the role of lateral fluorine substituents by synthesising and studying a series of mesogens with different substitution patterns.

We discovered that the formation of smectic phases is driven by significant differences in the variation of electron density between the ends of the molecule, while more uniform distribution of electron density suppresses smectic behaviour. For an intermediate case, the heliconical N$_{TBF}$ phase was observed. The physical properties of the polar phases were investigated, including the response of the SmA$_F$ and SmC$_F$ phases to an electric field. In both phases, the polarisation is large, ca. 4-5 μC cm^{-2}, and the primary driving mechanism of polarisation switching is the reorientation of layers, with the polarisation vector aligning with the electric field. However, in the SmC$_F$ phase, an intermediate step is observed during this process. The dielectric response of the smectic phases also differs significantly.

References

1 H. Kikuchi, H. Matsukizono, K. Iwamatsu, S. Endo, S. Anan and Y. Okumura, *Advanced Science*, 2022, **9**, 2202048.

2 G. J. Strachan, E. Górecka, J. Szydłowska, A. Makal and D. Pociecha, *Advanced Science*, 2025, **12**, 2409754.

Acknowledgments

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Transformations and Interactions of Point defects on a String of Half-Skyrmion

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Topological defects—localized regions of order singularity—are ubiquitous in systems ranging from cosmology to condensed matter and biology. Liquid crystals provide an ideal platform for visualizing such defects. However, three-dimensional defects, especially when they are riding on another topological structure, are much less characterized. Here we introduce a theoretical framework to describe point defects in an otherwise uniform nematic and on a string of half-skyrmion. We discuss how radial hedgehog and hyperbolic defects can continuously transform into each other. Our classification of point defects on a half-skyrmion are confirmed in the experiment. Moreover, elastic interactions between point defects on the half-skyrmion can exhibit highly tunable interactions. Our theoretical results not only advance the understanding of defects in nematic liquid crystals but also provide a general approach for characterizing topological structures in other partially ordered systems.

Liquid crystal skyrmions in external flows

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Liquid crystal (LC) skyrmions are topologically protected spatially-localised distortions of the director field which exhibit particle-like properties. Here, we investigate using experiments, numerical simulations and perturbative analysis effects of external flows on the structure and dynamics of LC skyrmions. Surprisingly, they exhibit qualitatively different behaviour depending on the origin of the flow: pressure driven or shear flow. In the former case, we find striking flow driven elongation of an isolated skyrmion and flow alignment of skyrmions within their assemblies. Simulations also reveal a somewhat surprising plastic response at very short times, which may be relevant in applications based on the alignment of soft structures such as LC skyrmions. In contrast, for Couette flows we observe a Hall-like drift of skyrmions in the direction perpendicular to the shear plane. A perturbative analysis of the dynamic Ericksen-Leslie equations demonstrates that the chiral term of the elastic torque is the main mechanism behind the transfer of linear momentum into the transverse direction.

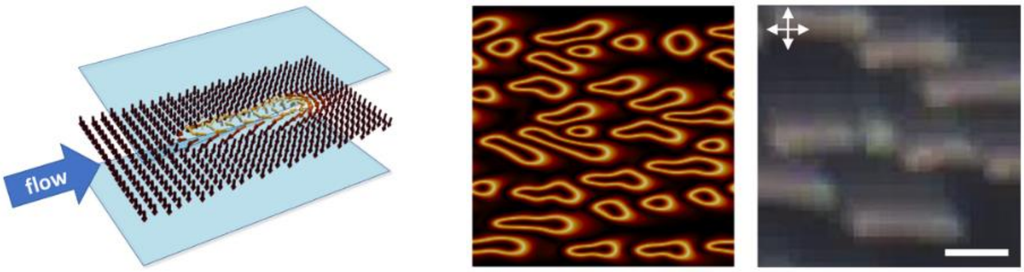

Figure: Elongation of liquid crystal skyrmions under external mass flow. (Left) Scheme, (middle) simulation of many skyrmions, (right) experiment, the scale bar is 50 µm.

Neutron scattering as a mesoscale probe for buried liquid crystals

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Confined liquid crystals (LCs) have garnered significant research interest due to their unique physical properties and promising applications. Various techniques, including dielectric, calorimetric, and optical methods, have been extensively used to study them. It has been found that mesoscale geometric confinement profoundly influences morphology and dynamics, leading to shifts in phase transition temperatures or even their complete suppression, depending on the confinement size and the elasticity of the host matrix [1].

Different porous materials can induce spatial confinement, such as anodic aluminum oxide, which provides 2D confinement through cylindrical channels [2]. Small-angle neutron scattering (SANS) was employed to investigate molecular ordering in cylindrical pores across a broad range of diameters for various LC materials. The findings confirm paranematic ordering near the boundaries of nanosized pores, whereas no ordering effects were detected in 200 nm pores. A paranematic layer of approximately 2-3 nm was identified. Additionally, neutron reflectometry (NR) was used to examine structural ordering in nematic and smectic LC thin films across a wide range of thicknesses, enabling a self-consistent structural description.

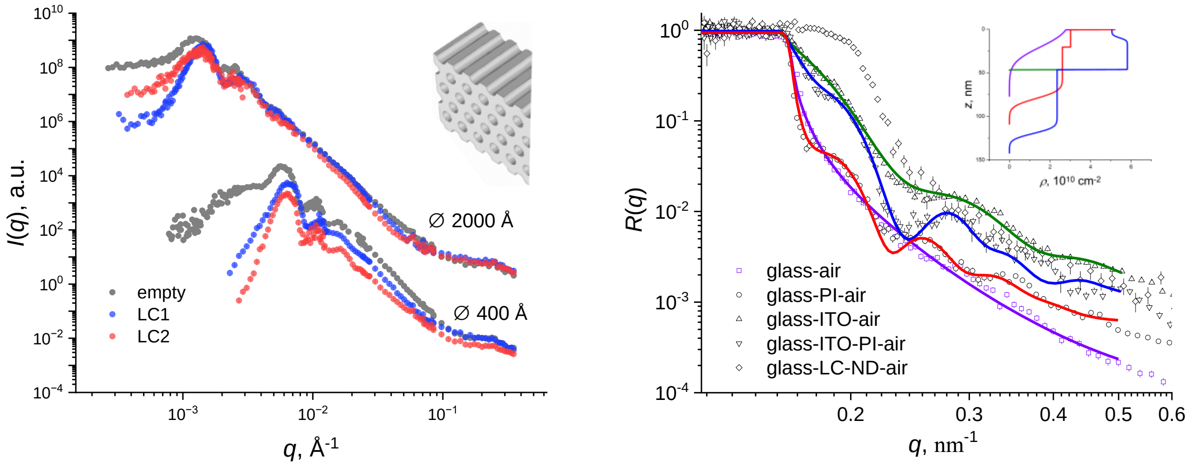

Fig. 1. Examples of SANS (left) and NR (right) applications to LC systems.

[1] M. Jasiurkowska-Delaporte *et al.*, *J. Mol. Liq.*, 2021, **331**, 115817.
[2] E. Juszyńska-Gałązka and W. Zając, *Phase Transit.*, 2023, **96**, 89-96.

Thermochromic Liquid Crystal Sensors for Ultrasound Visualisation Applications

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Ultrasonic field visualisation is used in non-destructive testing (NDT) to find and monitor defects in components. The standard visualisation method used is laser vibrometry, which is a scanning method offering high precision but using high cost equipment. A low cost method for visualising ultrasound, without scanning, would be beneficial for NDT applications. Thermochromic liquid crystal (TLC) sensors can be used to map ultrasound intensity on the surface of a sample[1]. Heat generated by ultrasonic fields is absorbed by the TLC film with the aid of a backing layer, altering the pitch of chiral nematic LC inside and changing the wavelength of reflected light. This wavelength is determined from optical photographs of the sensor and analysed to produce temperature maps of the surface comparable to ultrasound intensity[2]. Temperature corresponds to several factors including displacement, environment, and thermal conductivity of the sample.

The resolution limitations of the TLC sensors have been investigated by considering backing layer thickness and thermal conductivity, using modelling and experiments. Increasing backing layer thickness increases sensitivity, but reduces resolution. The sensors were also tested for defect detection applications. Surface defect detection and visualisation was demonstrated using different sized slots in a plate, showing that ultrasonic guided waves propagating along the defect generated non-uniform heating within the slot. Image analysis was conducted and the results were compared to modelling of wave propagation in the samples with slot defects.

1 Y. Kagawa, et. al, *J. Sound Vib*, 1974, **36**(3), 407-IN6.
2 M. Turvey, et. al, *Ultrasonics*, 2024, **141**, 107352.

Atomistic simulations of CB6OIBeOn: a progress report

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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→N→NTB→HexI→K (crystal) whereas for $n > 6$, the sequence was I→N→SmA→SmAB→ SmCTB→HexI→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 1536 molecules, using the the General AMBER Force Field (GAFF)[3], at a pressure of 1 bar.

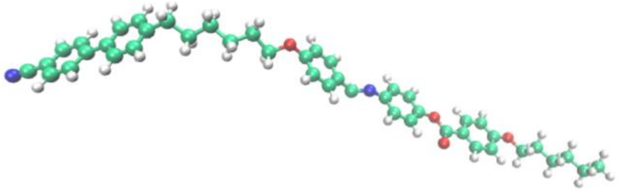

Figure 1: Molecule structure of CB6OIBeO$_6$

To date we have observed the nematic phase N and the twist-bend nematic phase N_{TB} for $n = 6$, as shown in Figure 2. And we also get Smectic A and the twist-bend Smectic C phase for n=7.

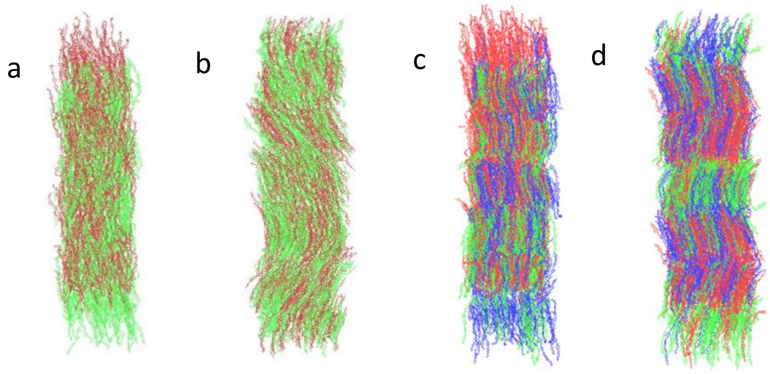

Figure 2: Simulation snapshots of CB6OIBeO$_6$, CB6OIBeO$_7$: (a) shows a nematic phase at 480K and (b) shows a twist-bend nematic phase at 400K (c) presents a smectic A phase at 395K and (d) presents a twist-bend Smectic C phase at 380K with different angle colouring between the long axis of molecules and y axis. The colouring reflects the ordering of the long axis of the molecules along the director.

Reference:

[1] Abberley, J. P. et al. Heliconical 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).

Posters

Effect of Monosaccharides and Disaccharides on the Structural Colour and Self-Assembly of Cellulose Nanocrystal Films.

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Cellulose nanocrystals (CNCs) self-assemble into lyotropic chiral nematic (cholesteric) liquid crystalline phases, forming helicoidal photonic films on evaporation that exhibit structural colour via Bragg reflection. This study investigates how mono- (glucose, fructose) and disaccharides (sucrose, inverted sugar) influence the optical response and phase behaviour of CNC suspensions and films, aiming to enhance reproducibility and tunability in bio-based photonic materials. CNC–sugar films were cast under controlled humidity (90%) and temperature (20 °C), as well as ambient conditions, and analysed for spectral shifts, colloidal stability (zeta potential: −51.8 to −76.9 mV), size distribution, and pitch evolution. Sugars induced a concentration-dependent redshift in reflected colour (460–895 nm) by expanding the chiral nematic pitch (p). This modulation arises from (i) chiral interactions, i.e. left-handed CNCs doped with right-handed sugars unwinding the helicoidal structure, and (ii) viscosity enhancement, which delays kinetic arrest, the transition from the ordered liquid crystalline phase to a rigid helicoidal structure during drying. Disaccharides, especially inverted sugar, caused the most pronounced redshifts and pitch broadening due to synergistic effects from hydrogen bonding and chirality. Polarized optical microscopy and RGB analysis showed that sugar concentrations above 22% w/w led to broader reflection bandwidths (FWHM up to 249 nm), indicating domain heterogeneity and reduced structural order. These findings demonstrate that the molecular properties of sugars, specifically their chirality and ability to modulate viscosity, can precisely tune both the structural colour and phase transition dynamics of CNC photonic films, offering new pathways for designing sustainable, tuneable optical materials for lasers, sensors, and photonic devices.

The Flexoelectric Instability in Nematic Liquid Crystals

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This study explores the theoretical model of the flexoelectric instability in nematic liquid crystals, composed of bent-core molecules, focusing on the coupling n between elastic deformations and applied electric field via the flexoelectric polarization. The theory of the flexoelectric instability is developed in the nematic phase just above the transition into the twist-bend phase, and thus, we take into account strong temperature variation of the flexoelectric coefficients and softening of the bend elastic constant determined by large flexoelectric corrections. By integrating elasticity theory and the theory of flexoelectricity in the framework of Landau de Gennes theory, the threshold conditions for instability are derived by minimization of the total free energy in the presence of the external electric field using the Euler-Lagrange equations. Assuming that the two of the elastic constants are equal ($K_1 = K_2 = K$), we simplify the model, which enables one to obtain the analytical solutions where the critical electric field and the wave vector of the periodic structure are determined. MATLAB simulations illustrate the relationship between the threshold field, temperature, dielectric anisotropy, and elastic constants. These visualizations highlight the role of thermal variations in triggering instability, providing insight into material behaviour. This framework bridges theoretical analysis with practical applications, aiding future experimental validations and liquid crystal technologies.

Towards the theory and simulation of the ferroelectric nematic phase

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For many liquid crystalline phases, simple models exist that allow one to develop a deep, insight into the properties of such phases. For example, hard spherocylinders exhibit nematic and smectic-A phases[1], while hard discs form a discotic nematic phase and a columnar phase[2]. The simplicity of such models permit extensive simulation studies and the development of quantitatively accurate statistical mechanical theories. Experimentally, colloidal particles with such shapes have also been shown to spontaneously form such phases[3]. We aim to find similar, simplified particle models that exhibit the ferro-electric nematic phase, taking inspiration from the work done by Madusudana[4] and the arguments made by Osipov[5]. In particular, we will study systems of hard spherocylinders, with embedded sites along the long axis. The interaction potential between these sites can be of varying magnitude and sign, thus providing a model closely related to the charge-wave model of Madusudana. We anticipate that a systematic study on this system will allow for the development of simple models that form the ferro-electric nematic phase and which may even inspire the synthesis of colloidal models, allowing for experimental investigation. Given the relative simplicity of the model, we also anticipate the development of semi-quantitative theory base, for example, on excluded volume theories previously developed for hard particle models.

1 S. C. McGrother, D. C. Williamson and G. Jackson, *The Journal of Chemical Physics*, 1996, **104**, 6755–6771.
2 S. Chandrasekhar and G. S. Ranganath, *Rep. Prog. Phys.*, 1990, **53**, 57–84.
3 R. J. Bushby and O. R. Lozman, *Current Opinion in Colloid & Interface Science*, 2002, **7**, 343–354.
4 N. V. Madhusudana, *Phys. Rev. E*, 2021, **104**, 014704.
5 M. A. Osipov, *Liquid Crystals Reviews*, 2024, **12**, 14–29.

Micro-Rod Particle Dynamics in the Nematic Phase of Liquid Crystals Under Electric Fields

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Liquid crystals (LCs) have a wide variety of applications, propelling them to the forefront of electro-optics and displays. In many recent applications, the behavior of liquid crystals depends on particles suspended within them. However, the behavior and distribution of these particles 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, alter their translational direction, and even affect their spatial organization [1] . Polarizing microscopy enables the examination of alignment quality and facilitates the identification of the electric field-frequency stability regimes where specific particle behaviors are observable [2] . Investigating micro-rods with different aspect ratiosleadsto a wealth of additional degrees of freedom for motion as compared to the translation observed forspherical particles[3] . Insight into their behavior is crucial for engineering novel materials and devices with specific features to diverse applications. The significance of aspect ratios in influencing the dynamic behavior of micromaterials in various settings is investigated in this work. Our experiments have unveiled novel modes of motion, encompassing both linear and nonlinear dynamics, for rod-shaped particles in a nematic liquid crystal under the influence of an electric field. The observed behaviors included linear translation, circular motion, and a newly characterized pattern involving rotation around both the long and short axes of the rods, obviously absent for spherical microparticles. Additionally, we identified novel macroscopic modes of motion, such as looping and logarithmic spiral trajectories. The dynamic behavior depends on particle size, confining cell gap, viscosity via temperature change, and electric field amplitude and frequency. The molecular boundary conditions produced by various cell gaps can alter how the particle in the liquid crystal reacts to outside stimuli, i.e. electric fields in our case. The results are of importance to fundamentally understand the motion of particle of different shape.

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

Understanding the Charge Transport Properties of Low-Symmetry Discotic Molecules

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Discotic liquid crystals – formed by disc-like molecules typically comprising a rigid aromatic core with flexible peripheral substituents – in their columnar phase are promising organic semiconductors for their attractive charge transport properties.[1-3] Discotic molecules therefore provide exciting model systems for developing fundamental understanding of charge transport as well as for the optimal design for opto-electronic applications.[1-3] For the ease of synthesis, discotic molecules mostly contain a highly symmetric aromatic core,[3] which has been found conducive to good charge transport properties.[4] However, low-symmetry discotic molecules can have attractive photophysical properties,[5] often warranting a trade-off between photophysical and charge transport properties for optimal opto-electronic applications via molecular design. The charge mobility is determined by the transfer rate (k_{ET}), which can be theoretically predicted by the Marcus theory within a thermally activated hopping formalism, and controlled by two key parameters, namely the transfer integral and the reorganization energy.[6,7] In this poster, we present preliminary results of our ongoing computational study to illustrate how the transfer integral critically depends on the molecular arrangements of certain recently synthesised low-symmetry discotic molecules and interpret our results by analysing relevant molecular orbitals. We will discuss how the understanding that we develop in this study can be exploited for the rational design of low-symmetry discotic molecules for attractive opto-electronic applications.

References

1. T. Wöhrle *et al.*, *Chem. Rev.*, 2016, **116**, 1139–1241.
2. B. R. Kaafarani, *Chem. Mater.*, 2011, **23**, 378–396.
3. S. Sergeyev, W. Pisula and Y. H. Geerts, *Chem. Soc. Rev.*, 2007, **36**, 1902–1929.
4. X. Feng, V. Marcon, W. Pisula, M. R. Hansen, J. Kirkpatrick, F. Grozema, D. Andrienko, K. Kremer and K. Müllen, *Nature Mater.*, 2009, **8**, 421-426.
5. J. A. Rego, S. Kumar and H. Ringsdorf, *Chem. Mater.*, 1996, **8**, 1402-1409.
6. R. A. Marcus, *Rev. Mod. Phys.*, 1993, **65**, 599-610.
7. E. F. Valeev, V. Coropceanu, D. A. da Silva Filho, S. Salman and J.-L. Brédas, *J. Am. Chem. Soc.*, 2006, **128**, 9882-9886.

Simulations of liquid crystal tactoids and elastomers

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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 using the Morpho software[2].
The initial mesh is initialised with a homogenous director field. The one elastic constant approximation is used in which $K1=K2=K3=K=1$ and anchoring strength is varied in the range 0 to 10, as per Prinsen paper [1]. To advance to the 3D simulation of tactoids the 2D initial mesh was replaced by a 3-dimensional mesh. Our results of aspect-ratio and total energy are finding excellent agreement and validating the simulation methods adopted.
To expand the possibilities of Morpho, we utilized the linear elasticity module in built in the software which can control poisson's ratio and lame coefficients. By applying a uniform force field on an elastomer sheet, we tried to stretch it and relax back into original form to test elasticity. Further steps will aim to model and study the stress-strain behaviors of elastomers with different configurations and incorporate anisotropic charcteristics.

References

1. Prinsen, P., & Van Der Schoot, P. (2003). Shape and director-field transformation of tactoids. *Physical Review E*, *68*(2), 021701.
2. Joshi, C., Hellstein, D., Wennerholm, C. *et al.* A programmable environment for shape optimization and shapeshifting problems. *Nat Comput Sci* **5**, 170–183 (2025).

Design and characterisation of Blue Phase Adaptive Optics correctors

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Adaptive optics is a technique used to reduce the phase distortion introduced by the propagation medium in a free space optical system. This was first developed for Astronomy1 , but now finds applicability in Microscopy, Ophthalmology, and Communications. 2 In the case of Astronomy and Earth-to-satellite communications, the propagation medium introducing aberration is the lowest layer of the atmosphere, the Troposphere. This is because air of various temperatures is being pushed around by wind, leading to changes in local refractive index, and thus distorted wavefronts.

Crucially, the rate at which these effective refractive index changes happen is approximately 1000 times per second.3 This requires correction devices which can operate at this speed. Liquid Crystals are commonly found within Microscopy and Ophthalmology as Adaptive Optics correctors, where the samples or the movement of the human eye do not require sub-millisecond response times.2 This work describes the performance of a novel Blue Phase correcting device which may withstand the requirements of atmospheric turbulence.

In this paper, the process of obtaining large area correcting devices will be described, using monodomain growth techniques (slow cooling rate, thermal cycling, electrostriction), stabilisation (UV photopolymerisation) and LCoS (Liquid Crystal on Silicon) backplane fabrication. Progress on this device design will be presented, including design considerations for atmospheric turbulence correction. The backplane is tailored for Adaptive Optics, chosen to match the wavefront sensor 1:1. The device is to be placed in the conjugate plane of this sensor and tested for its ability to modulate light at kHz rates, with results to be presented.

References

1. G. Rousset, J.C. Fontanella, P. Kern, P. Gigan, F. Rigaut, P. Léna, C. Boyer, P. Jagourel, J.P. Gaffard and F. Merkle, Astronomy and Astrophysics, 1990, 230, L29-L32.
2. K.M. Hampson, R. Turcotte, D.T. Miller, K. Kurokawa, J.R. Males, N. Ji and M.J. Booth, Nature Reviews Methods Primers, 2021, 1, 68.
3. P. Wizinowich, Contemporary Physics, 2015, 56:4, 432-450.

Deep Learning Driven Design of Novel Ferroelectric Nematic Liquid Crystals

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The scarcity of known compounds exhibiting a ferroelectric nematic (N_F) phase[1-4] is a limiting factor in the development of the field. Traditional lab-based synthesis of compounds is a time-consuming and resource intensive process. Here we present an alternative deep learning-based approach for generating novel molecules with predicted N_F transitions.

Our approach utilises an experimental dataset of computer readable molecular structures and their associated liquid crystal transition temperatures. This dataset is curated from all presently disclosed N_F materials in the publication and patent literature, as well as unpublished materials from our group. We employ a variational autoencoder[5] model trained on a graph representation of the molecular structural information to generate novel molecular structures. A rule-based application of both a molecular graph classifier and a molecular graph property predictor produces a pool of N_F molecules with predicted N_F transition temperatures. By integrating computational retrosynthesis techniques[6] we further filter the N_F pool into readily synthesisable molecules, bridging the gap between computational predictions and laboratory-based chemistry. This is interfaced with a digitised laboratory inventory for our group which enables us to discriminate targets based on the availability of precursors This work is a step towards the discovery of a single-compound room temperature N_F material but also has potential for broader applications in liquid crystal research with regards to designing for specific properties

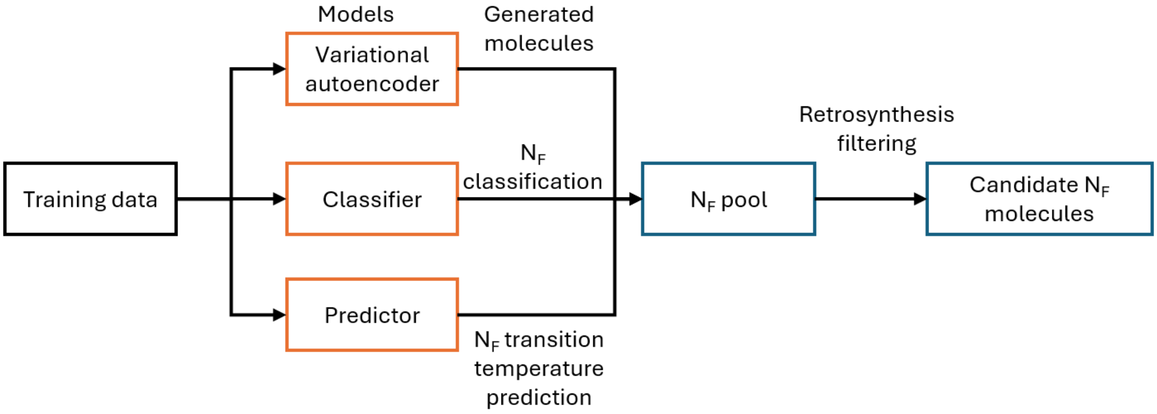

Figure 1. Deep learning-based workflow to generate candidate N_F molecules.

References

1. R. J. Mandle, S. J. Cowling and J. W. Goodby, *Chemistry – A European Journal*, 2017, **23**, 14554-14562.
2. R. J. Mandle, S. J. Cowling and J. W. Goodby, *Physical Chemistry Chemical Physics*, 2017, **19**, 11429-11435.
3. H. Nishikawa, K. Shiroshita, H. Higuchi, Y. Okumura, Y. Haseba, S. I. Yamamoto, K. Sago and H. Kikuchi, *Advanced Materials*, 2017, **29**.
4. X. Chen, E. Korblova, D. P. Dong, X. Y. Wei, R. F. Shao, L. Radzihovsky, M. A. Glaser, J. E. Maclennan, D. Bedrov, D. M. Walba and N. A. Clark, *Proceedings of the National Academy of Sciences of the United States of America*, 2020, **117**, 14021-14031.
5. M. Lee and K. Min, *Journal of Chemical Information and Modeling*, 2022, **62**, 2943-2950.
6. S. Genheden, A. Thakkar, V. Chadimová, J.-L. Reymond, O. Engkvist and E. Bjerrum, *Journal of Cheminformatics*, 2020, **12**, 70.

The Twist-Bend Smectic Phases: On the Role of Lateral Substituents

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One of the newest classes of liquid crystal phases discovered are the twist-bend phases, observed in achiral, bent-shaped dimers: the twist-bend nematic (N_{TB}) phase, first experimentally observed in 2007 in the symmetric dimer CB7CB [1], and more recently, in 2017, the twist-bend smectic (SmC_{TB}) phases in homologues of non-symmetric dimers such as the CT6O.*m* series with long terminal chain *m* [2]. Since the discovery of these phases, significant research has been dedicated to understanding the structure-property relationships which govern their formation. This has included the synthesis of several new series of dimers with structural changes to the nature and size of mesogenic groups, the central spacer, and the terminal chains. One such modification to the CT6O.*m* series (Figure 1(a)) was the addition of a lateral methyl branch on the benzylideneaniline mesogenic unit, giving the CT6O2Me.*m* series (Figure 1(b)) [3]. Homologues with a long terminal chain *m* showed twist-bend smectic behaviour, namely the previously reported interdigitated $SmC_{TB\text{-}SH}$ and $_{\text{-}DH}$ phases, however those with short *m* exhibited a new variant of the SmC_{TB} phase: an apparently heliconical, intercalated smectic phase with a temperature-dependent pitch length, here termed $SmC_{TB\text{-}X}$.

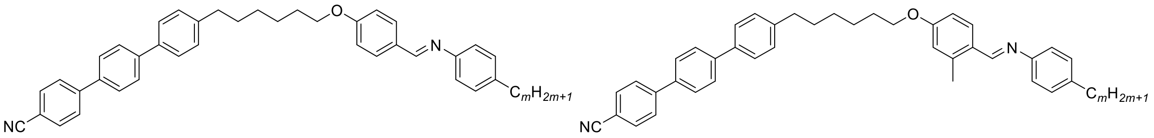

Fig. 1: (a) Molecular structure of the CT6O.m series. (b) Molecular structure of the CT6O2Me.m series.

In the present work, we report new series of liquid crystal dimers based on the structure of CT6O2Me.*m* in which the size, position and chemical nature of the lateral branch is varied. It appears that these variables have a strong effect on molecular packing into, and thus the stability of, the intercalated $SmC_{TB\text{-}X}$ and other twist-bend phases.

[1] Cestari, M. *et al. Phys. Rev.* E, 84, 031704, (2011)
[2] Walker, R. *et al. J. Mater.Chem. C*, 9, 5167-5173, (2021); Abberley, J.P. *et al. Nat. Commun.*, 9(1), 228, (2018).
[3] Alshammari, A., Pearson, A. *et al. Manuscript in preparation*, (2025).

Synthesis and Characterisation of Highly Fluorinated Ferroelectric Nematogens

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The ferroelectric nematic phase, NF, has been of significant research interest since its discovery in two different materials that were independently published in 2017: RM734[1] and DIO[2]. The NF phase has demonstrated a host of unprecedented and highly desirable electronic and optical properties, including extraordinarily high polarisation values, and dielectric anisotropies several hundred times larger than those of conventional nematogens[1-3]. RM734 and DIO, as well as the subsequently discovered UUQU-4N[4], are considered the archetypal structures that the vast majority of ferroelectric nematic liquid crystals are based on to date. However, while upwards of 300 molecules have been investigated to date, it is still not yet well understood what combination of features best support the appearance and stability of the NF phase. We aim to deepen this understanding of the structure-property relationships underpinning this fascinating phase of soft matter through the synthesis and characterisation of new ferroelectric nematogens.
In the present work, we combine some of the characteristic chemical motifs of DIO-type and UUQU-type structures to create new ferroelectric nematogens with a highly fluorinated mesogenic core. We compare multiple series of molecules based on this core, varying both fluorination patterns and terminal chain lengths on the dioxane ring in order to evaluate the effect of these structural features on the appearance and stability of the ferroelectric nematic phase.

[1] R. J. Mandle, S. J. Cowling, J. W. Goodby, *Chem. A Eur. J.*, 2017, **23**, 14554–14562.
[2] H. Nishikawa, K. Shiroshita, H. Higuchi, Y. Okumura, Y. Haseba, S. I. Yamamoto, K. Sago, H. A. Kikuchi, *Adv. Mater*., 2017, **29**, 1702354.
[3] F. Caimi, G. Nava, R. Barboza, N. A. Clark, E. Korblova, D. M. Walba, T. Bellini, L. Lucchetti, *Soft Matter*, 2021, **17**, 8130–8139.
[4] A. Manabe, M. Bremer, M. Kraska, *Liq. Cryst*., 2021, **48**, 1079–1086.

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