BLCS
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Joint Conference of the British & German Liquid Crystal Societies

University of Edinburgh, 21-23 March, 2016

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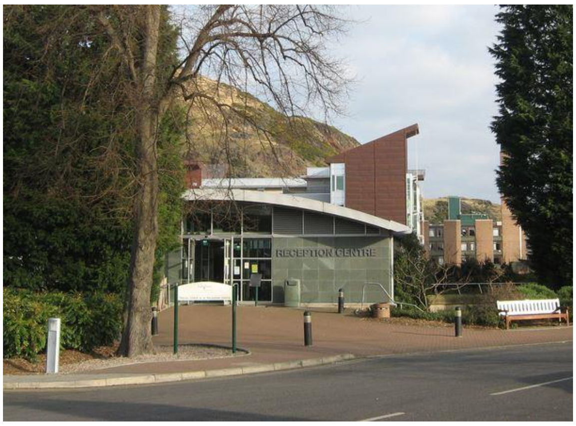
Welcome from the conference chairs

Welcome to the first joint conference of the British Liquid Crystal Society (BLCS) and the German Liquid Crystal Society (DFKG), held at the University of Edinburgh, 21-23 March, 2016.

The conference is located on the first floor of the John McIntyre Conference Centre (JMCC), on the Pollock Halls Campus of the University of Edinburgh, about 1 to 2 miles (a short taxi or bus ride) from Edinburgh City Centre and nestling at the foot of Arthur's Seat. Entrance to the Pollock Halls campus is via the Holyrood Park Road entrance. Close to this entrance, you will also find the Edinburgh First Reception Centre, for all enquiries related to University-owned facilities/accommodation, tourist and travel information, and booking of taxis.



Left: Edinburgh First Reception Centre, Pollock Halls (for University-owned accommodation).
Right: John McIntyre Conference Centre (location of all conference sessions).

Free WiFi is available throughout the JMCC (SSID: **keysurf**). Note that this will work for 24 hours at a time only, and so will require re-registering each day. Alternatively, for those who are able to use it, the **Eduroam** WiFi system is also available throughout the University of Edinburgh.

Oral presentations will be held in the Pentland East room. If you are a speaker, please use the various lunch/coffee breaks to upload and check your presentation in advance of your session, and also to make yourself familiar to your session chair. You may use your own laptop if you prefer. Please keep strictly to the speaker timetable, and use the radio microphones provided.

Poster presentations will be held in the Pentland West room. There are 2 poster/exhibition sessions, on the Monday and Tuesday evenings. Please ensure your poster is put up before 5:30pm on Monday evening in time for the first poster session. Please also remove your poster by 7:00pm, after the Tuesday session is completed.

Thank you again for taking the time to attend the conference. We hope you enjoy the programme! A full-colour PDF of these proceedings can also be downloaded from our website: blcs2016.eng.ed.ac.uk/programme.

Dr Philip J.W. Hands, University of Edinburgh

Prof Matthias Lehmann, University of Würzburg

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Please take the time to visit our exhibitors during your breaks and the poster sessions. We express sincere thanks to our sponsors, without whose invaluable support, this conference would not have been possible.

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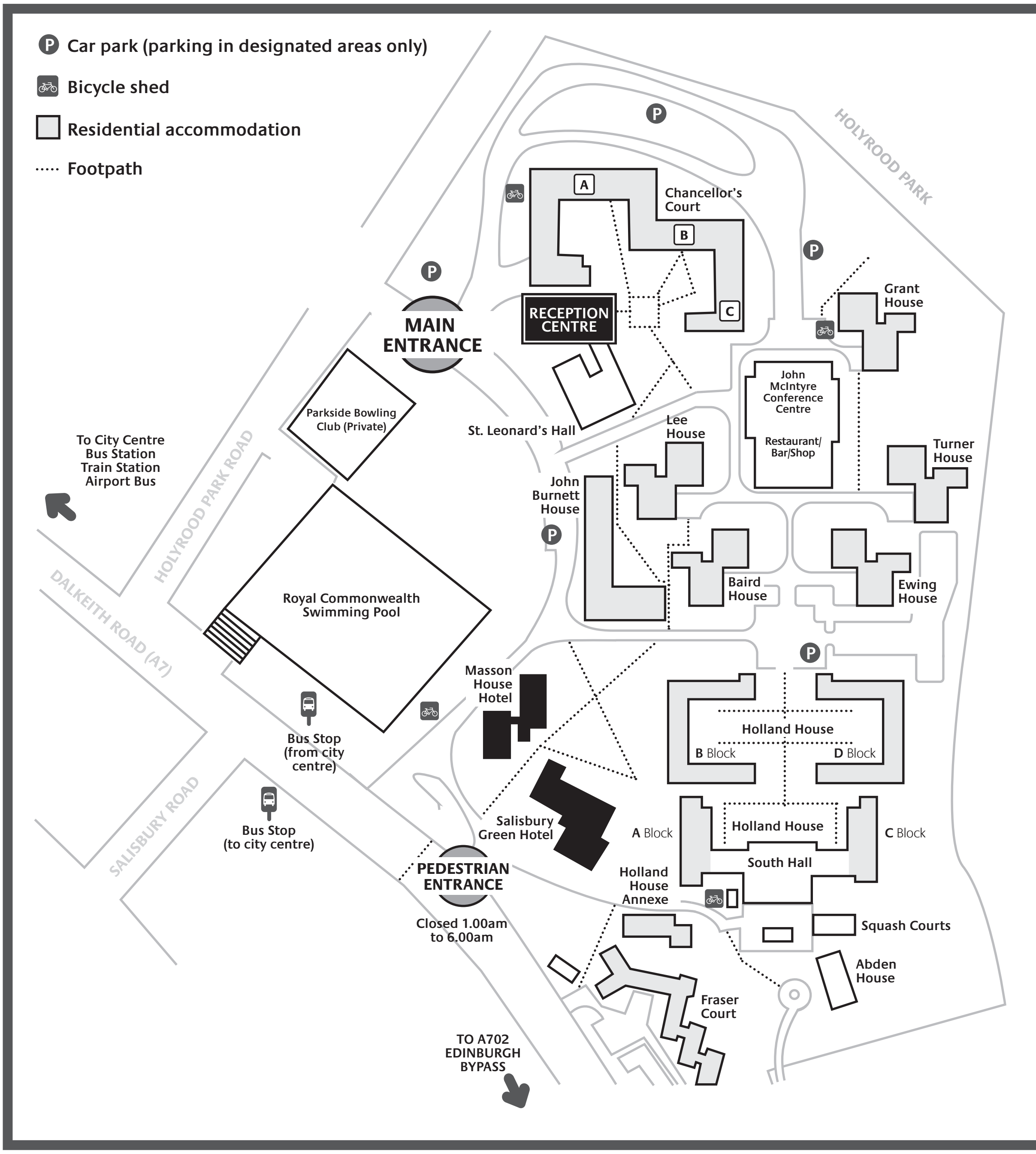

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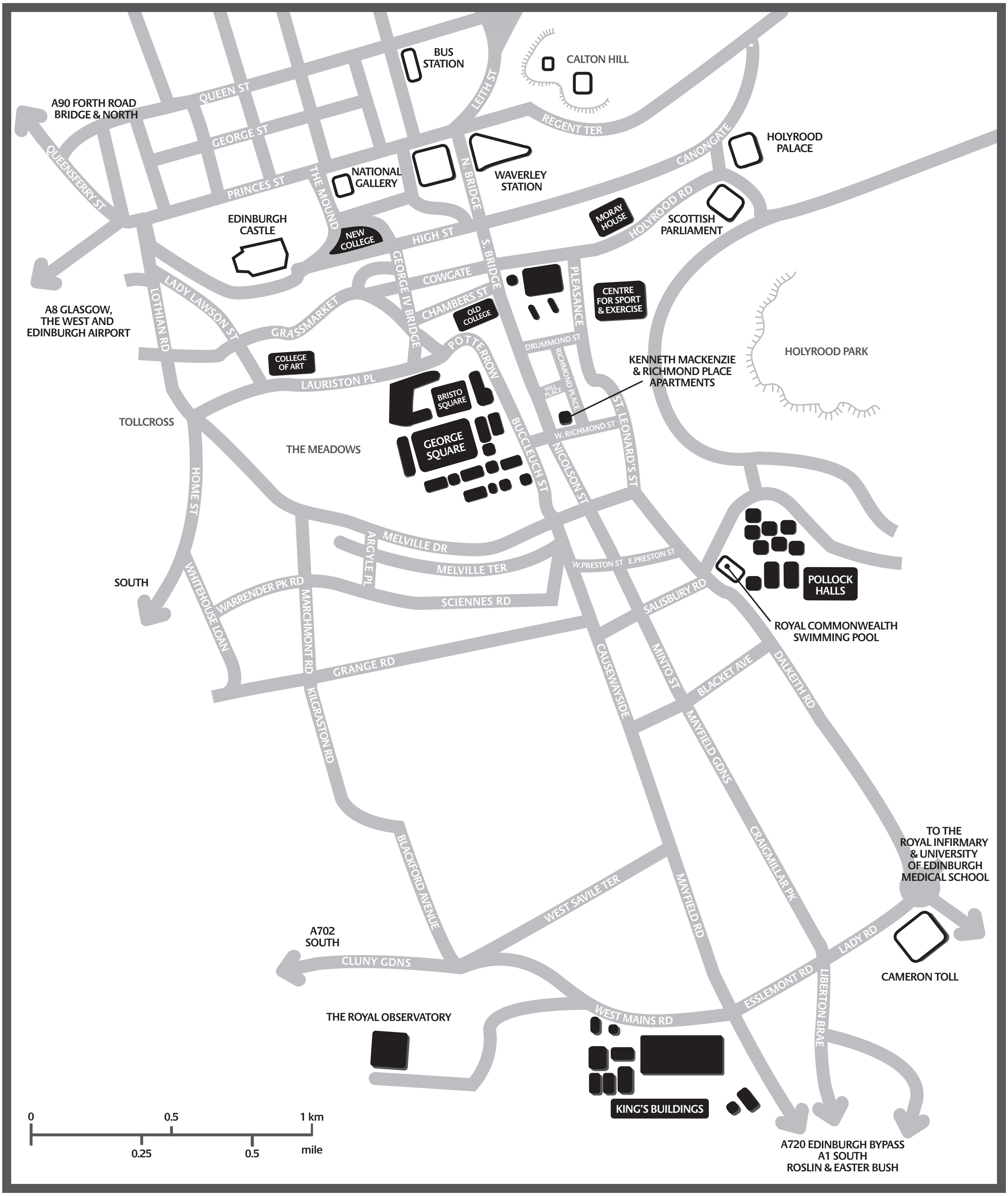


Conference programme

DAY 1: Monday 21 March

11:00	JMCC 1st floor foyer	Registration			
12:30		Lunch			
13:30	Pentland East	Welcome from conference chairs, Philip Hands & Matthias Lehmann			
Session 1: Chair: Andrew Masters					
13:45	Pentland East	I1	Wilson Poon	University of Edinburgh	Ben Sturgeon Lecture: *The universe in a bacterial colony: growing E.coli as active nematics*
14:35	Pentland East	O1	Ingo Dierking	University of Manchester	*Liquid crystal - ferrofluid dispersions*
14:55	Pentland East	O2	Alexander Lorenz	University of Paderborn	*Polymer enhanced LCs with continuous optical phase modulation*
14:55	Pentland East	O3	Daniel Svenšek	University of Ljubljana	*Proposing a generalized conservation law for main-chain polymer nematics*
15:15		Tea/coffee			
Session 2: Chair: Frank Gießelmann					
15:45	Pentland East	O4	Simon Siemianowski	Merck KGaA	*Liquid crystal technologies towards realising a Field Sequential Colour (FSC) display*
16:05	Pentland East	O5	Mark Sims	University of York	*Rationalising dye alignment in liquid crystal hosts through a combined experimental and computational approach*
16:25	Pentland East	O6	Joachim Vollbrecht	University of Paderborn	*Liquid crystalline and spectroscopic properties of distorted arene cores*
16:45	Pentland East	O7	Martin Walker	University of Durham	*Persistence length of chromonic aggregates*
17:05	Pentland East	O8	Claudia Schmidt	University of Paderborn	*Order parameters from 1H NMR using the Haller extrapolation*
17:25	Pentland West	Poster session, exhibition and evening food/drink reception			
20:00	JMCC bar	Further networking opportunities			

DAY 2: Tuesday 22 March

08:30	Centro	Tea/coffee			
Session 3: Chair: Ralf Stannarius					
09:00	Pentland East	O9	Pascal Cachelin	Queen Mary University of London	*Sensing potential: the use of chiral nematic thin films incorporating reactive chiral dopants as sensors*
09:20	Pentland East	O10	Jürgen Schmidtke	University of Paderborn	*Using absorption bands for photonic band gap engineering in cholesteric liquid crystals*
09:40	Pentland East	O11	Jennifer Jones	University of Cambridge	*Modelling of free-standing perovskite-chiral polymer film structures for lasing*
10:00	Pentland East	O12	Oliver Henrich	University of Edinburgh	*Poiseuille flow of cholesteric liquid crystals*
10:20		Tea/coffee			
Session 4: Chair: Helen Gleeson					
10:50	Pentland East	I2	Maria Godinho	Universidade Nova de Lisboa	BLCS Visiting Lecturer: *Micro-filaments decorated by liquid crystal droplets*
11:40	Pentland East	O13	Tristan Hessberger	University of Mainz	*Liquid crystalline actuating Janus-particles by a co-flow microfluidic synthesis*
12:00	Pentland East	O14	Diana Khoromskaia	University of Warwick	*Dynamics of defects in shells of active liquid crystal*
12:20	Pentland East	O15	Martin Urbanski	University of Luxembourg	*Virtual polarising microscopy on nematic shells*
12:40		Lunch			
Session 5: Chair: Nigel Mottram					
13:40	Pentland East	I3	Randy Kamien	University of Pennsylvania	George Gray Medal Lecture: *Linking in liquid crystals*
14:30	Pentland East	O16	Efthymia Ramou	University of Hull	*Mesophase behaviour in dimeric systems with a nematic-nematic transition*
14:50	Pentland East	O17	Tino Reppe	University of Halle	*Mirror symmetry breaking in cubic and isotropic liquid phases of achiral polycatenar molecules*
15:10	Pentland East	O18	Mark Wilson	University of Durham	*Atomistic simulation of liquid crystals: towards the accurate prediction of phases and phase transition temperatures*
15:30		Tea/coffee			
Session 6: Chair: Corrie Imrie					
16:00	Pentland East	O19	Kirsten Harth	Otto von Guericke University, Magdeburg	*Retarded rupture of LC shells and bubbles in viscous environment*
16:20	Pentland East	O20	Giampaolo D'Alessandro	University of Southampton	*Multiscale models of freely rotating inclusions in nematic liquid crystals*
16:40		BLCS AGM (Pentland East) DFKG AGM (Prestonfield)			
17:40	Pentland West	Poster session, exhibition, networking			
19:00	South Hall	Conference dinner and awards			

DAY 3: Wednesday 23 March

08:30	Centro	Tea/coffee			
Session 7: Chair: Jan Lagerwall					
09:00	Pentland East	O21	Nikita Solodkov	University of Leeds	*Alignment and electro-optic properties of ferroelectric smectic C* liquid crystals with a direct transition to the nematic and isotropic phases*
09:20	Pentland East	O22	Marc Harjung	University of Stuttgart	*Electroclinic effect in a chiral lyotropic lamellar phase*
09:40	Pentland East	O23	Christopher Prior	University of East Anglia	*Probing lyotropic liquid crystal phases by a combination of EPR spectroscopy and molecular dynamics simulation*
10:00	Pentland East	O24	Frank Jenz	University of Stuttgart	*Orientational distribution functions and order parameters in "de Vries"-type smectics – a simulation study*
10:20		Tea/coffee			
Session 8: Chair: Georg Mehl					
10:50	Pentland East	I4	Andy Cammidge	University of East Anglia	Cyril Hilsum Medal Lecture: *Design and synthesis of new disc-like molecules that probe the limits for mesophase formation*
11:40	Pentland East	O25	Giusy Scalia	University of Luxembourg	*Self-assembled molecular wires of discotic liquid crystal formed with the crucial contribution of solvents*
12:00	Pentland East	O26	Markus Hügel	University of Würzburg	*New shape-amphiphiles self-assembling in filled columnar mesophases*
12:20	Pentland East	O27	Martin Horčic	UCT Prague	*Bent-core dimers utilizing benzenetriol central cores*
12:40		Lunch			
Session 9: Chair: Matthias Lehmann					
13:40	Pentland East	O28	Silvio Poppe	University of Halle	*Formation of new complex LC phases by T-shaped bolapolyphiles*
14:00	Pentland East	O29	Daniel Paterson	University of Aberdeen	*An isothermal twist-bend nematic to nematic phase transition*
14:20	Pentland East	O30	Tim Atherton	Tufts University	*Shape minimization problems for liquid crystals*
14:40	Pentland East	O31	Alf Martínez-Felipe	University of Aberdeen	*Towards supramolecular complexes showing the twist-bend nematic phase*
15:00	Pentland East	Prizes & final words from conference chairs, Philip Hands & Matthias Lehmann			
15:20		Tea/coffee			
		End of conference			

16:00 Holyrood *BLCS committee meeting*

The universe in a bacterial colony: growing *E. coli* as active nematics

Wilson C.K .Poon

School of Physics & Astronomy, University of Edinburgh, Edinburgh, UK

The study of 'active matter' has become very fashionable in condensed matter physics nowadays *[1]*. I will start by introducing the field in general, before homing in on bacteria as some of the simplest experimental realisations of active matter systems in the laboratory. After briefly surveying how motile bacteria behave as active matter, I'll focus on the apparently simple phenomenon of a single, immotile bacterium giving birth to daughter cells by binary fission. In particular, I will demonstrate how one could extend concepts learnt from the study of (passive) liquid crystals - nematic order, defects, etc. - to the description and elucidation of the process whereby a bacterial colony grows, initially in 2D, before buckling into the third dimension. An analogue to Hubble's Law for the universe-at-large will be established, and shown to be crucial to the emergence of new phenomena in a growing bacterial colony not so far observed in other active matter systems.

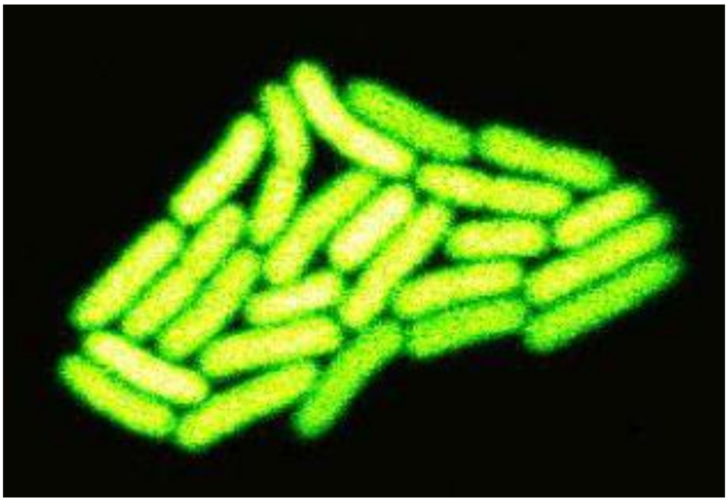


Figure 1. Optical micrograph of a growing colony of fluorescent *Escherichia coli* cells confined to the top of an agar gel by a glass cover-slide. Local nematic order as well as a nascent -1/2 defect at the top of the colony are clearly visible. Quantifying such liquid crystalline effects leads to a new description of this most basic form of living matter as an 'active nematic'. The scale is set by the width of each cell, which is about 0.8 μm.

I acknowledge Dario Dell'arciprete, Matthew Blow, Aidan Brown, Fred Farrell, Juho Lintuvuori, Alex McVey and Davide Marenduzzo for contributing to the results that I will be presenting in this lecture.

References

[1] M. C. Marchetti, J. F. Joanny, S. Ramaswamy, T. B. Liverpool, J. Prost, Madan Rao, and R. Aditi Simha
Rev. Mod. Phys. 85, 1143 (2013).

Micro-filaments decorated by liquid crystal droplets

Maria H. Godinho

CENIMAT/I3N, Departamento de Ciência dos Materiais, Faculdade de Ciências e Tecnologia, Universidade Nova de Lisboa, Caparica, Portugal

In a garden, early in the morning, spider webs can appear decorated with water droplets, and if the spider silk is adorned with nematic liquid crystal (LC) droplets? Can we get information about the morphology of the filaments from the structures of the LC droplets? In this work we try to address these questions. The first part of the talk will be dedicated to micro-filaments, their shapes and morphologies. The second part concerns the study of pierced liquid crystal droplets on diverse micro-filaments. The main objective is to probe the fibres' surface morphologies with LC droplets. This presentation represents part of the work published in refs *[1-3]* in which two major families of bio-fibres were used: filaments produced from isotropic or cholesteric solutions of cellulose and fibres collected from different species of spiders. The surfaces of the cellulosic fibres were found to induce unidirectional planar alignment, which was revealed to be axial for smooth achiral fibres and helicoidal for fibres produced from chiral liquid crystalline phases. The spider silks were collected from *Araneidae mangora*, *Latrodectus geometricus*, and *Pholcus phalangioides* spider webs. The spider silks observed showed to be achiral and to induce planar (Figure a.-c.) and homeotropic (Figure d.-f.) alignment. In this presentation the same method is also applied to the observation of some helical microfilaments present in plants *petiole trachearies*. The simple method used opens new horizons on the design of sensors, which can easily reveal bio-filaments' surface properties, comprising morphology and chirality.

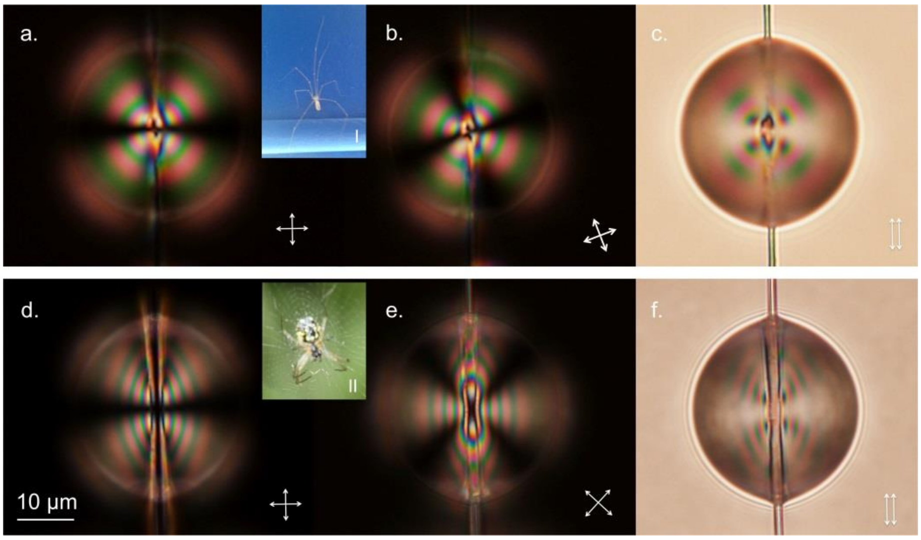


Figure 1: Nematic liquid crystal (NLC) droplets, with homeotropic anchoring at the droplet-air surface, pierced on spider silks. a.,b. and c. NLC droplet pierced on a filament produced by a *Latrodectus geometricus* (I) with planar anchoring at the droplet-fibre surface, under crossed (a. and b.) and parallel (c.) polarizers. d., e. and f. NLC droplet pierced on a fibre produced by an *Araneidae mangora* (II) with homeotropic anchoring at the droplet-fibre surface, under crossed polarizers (d. and e.) and parallel (f.) polarizers, in this droplet we can also notice the ellipsoidal fringes, which are typical for homeotropic anchoring on the fibre surface *[1]*.

References

[1] L.E. Aguirre, A. de Oliveira, D. Seč, S. Čopar, P.L. Almeida, M. Ravnik, M.H. Godinho, and S. Žumer, PNAS, 113(5), 1174-1179 (2016).

[2] Y. Geng, D. Seč, P.L. Almeida, O.D. Lavrentovich, S. Žumer, M.H Godinho, Soft Matter, 9(33), 7928-7933 (2013).

[3] Y. Geng, P.L. Almeida, J.L. Figueirinhas, E.M. Terentjev, M.H. Godinho, Soft Matter, 8(13), 3634-3640 (2012).

Linking in liquid crystals

Randall D. Kamien

Department of Physics and Astronomy, University of Pennsylvania, Philadelphia, USA

In addition to their ubiquitous use in technology, their profoundly beautiful images, and their rich phase behaviour, liquid crystals provide us with an arena to hone our understanding of geometry and topology. In this talk, I will discuss how knotting and linking manifest themselves in nematics and smectics and show that the same mathematics can be used to understand them. What goes around comes around.

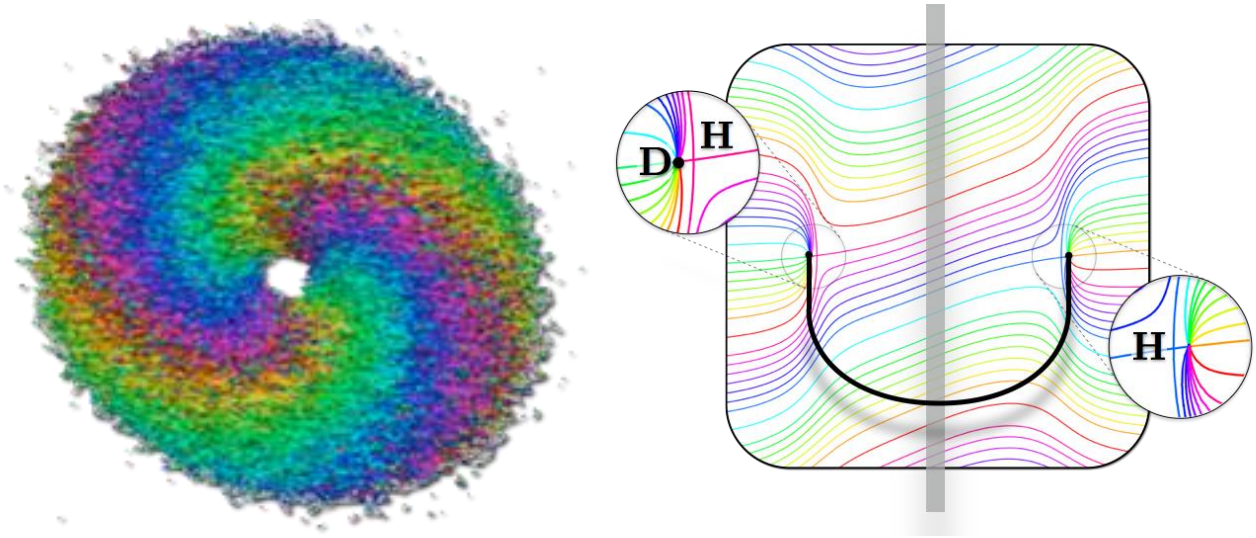


Figure 1. Left: Real data showing the Hopf Fibration in a Cholesteric. Right: Topological linking in smectics.

I am indebted to the students, postdocs, and faculty who have worked with me. This work, in particular, could not have been done without Gareth Alexander, Bryan Chen, Elisabetta Matsumoto, and Ricardo Mosna.

References

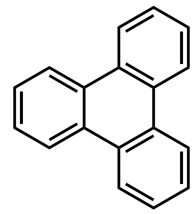
[1] R.D. Kamien and R.A. Mosna, arXiv:1510.07150.
[2] B.G. Chen, P.J. Ackerman, G.P. Alexander, R.D. Kamien, and I.I. Smalyukh, Phys. Rev. Lett. **110** (2013) 237801.

Design and synthesis of new disc-like molecules that probe the limits for mesophase formation

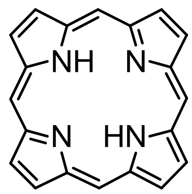
Andrew N. Cammidge

School of Chemistry, University of East Anglia, Norwich, UK

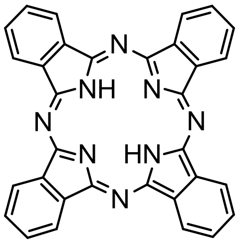
The chemistry of discotic liquid crystals has become a somewhat mature field, yet the interplay between design, synthesis and properties still highlights frequent surprises. In this talk the discotic liquid crystal cores under consideration are (sometimes loosely) based on triphenylene, porphyrin and phthalocyanine. Synthetic advances will be described that have opened the possibilities for both iterative and adventurous molecular design, allowing links between molecular structure and mesophase stability to be established.



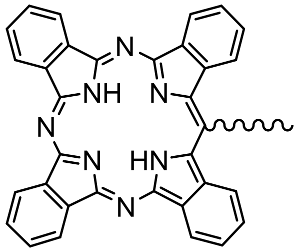
Triphenylene



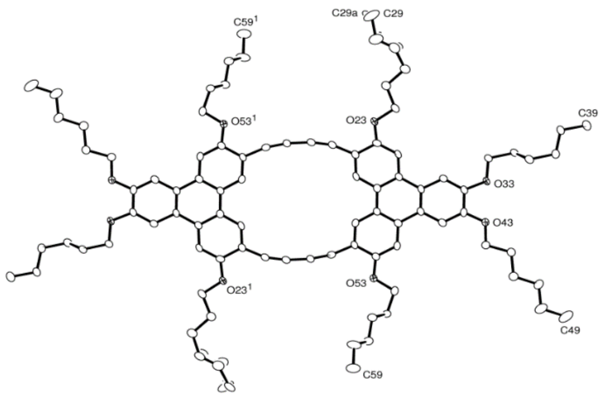
Porphyrin



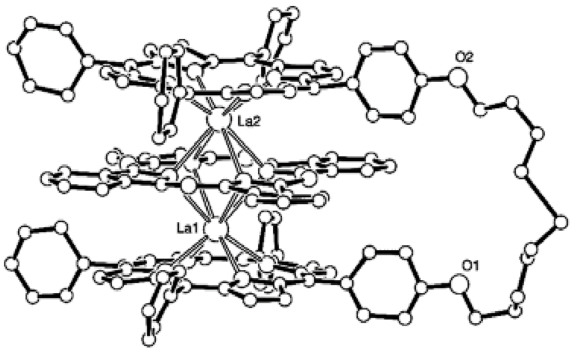
Phthalocyanine



Hybrids



Twins



Stacks

References

[1] (Triphenylenes) A. N. Cammidge, C. Chausson, H. Gopee, J. Li and D. L. Hughes, *Chem. Commun*. 7375-7377, (2009).

[2] (Twins) L. Zhang, H. Gopee, D. L. Hughes and A. N. Cammidge, *Chem Commun*. 46, 4255-4257, (2010).

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O1

Liquid crystal - ferrofluid dispersions

I. Dierking, T. Kelly, W. Pitcher

School of Physics and Astronomy, University of Manchester, Manchester, UK

Ferrofluids *[1]* are colloidal, nano-sized magnetic particles coated with a surfactant, which are suspended in an isotropic carrier fluid, often water or an organic solvent. A typical ferrofluid is composed of approximately 5vol % of particles, about the same amount of surfactant and the rest being the carrier fluid. They are known for their capability of pattern formation under magnetic field application, but it should be noted that they are not strictly ferromagnetic, i.e. they do not retain a magnetization when the field is turned off. Often, they are classified as superparamagnetic, because of their extremely large magnetic susceptibility. The applications of ferrofluids are to be found in material science, for example in the visualization of magnetic domain structures, as contrast enhancers for magnetic resonance imaging (MRI), as heat removers in high performance loudspeakers, or as liquid seals in hard drives.

Ferrofluids, dispersed in nematic liquid crystals, can form droplets of varying size, which are strongly responsive to the application of magnetic fields. In the field free state, nematic defects are formed in the vicinity of the droplets, which attract each other, and will lead to chaining of droplets. We thus have single droplets or chains of droplets dispersed in an anisotropic fluid (see fig. 1). These are not "ferronematics", but two-phase systems, where the ferrofluid inclusion reacts easily on application of a magnetic field.

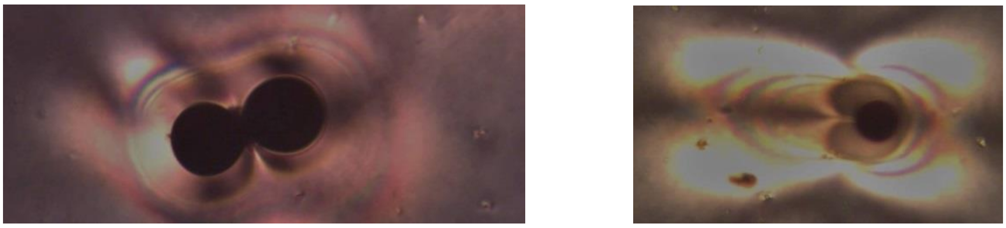

Figure 1. (left) Two ferrofluid droplets forming a chain, mediated via defects in the director field of the liquid crystal. (right) Ferrofluid droplet moving right, due to application of a magnetic field.

We have realized these systems and studied their properties. During this investigation a number of interesting fluid dynamic behaviour was observed. On magnetic field application the droplets initially repel from the magnet before they get attracted. Depending on the field strength, chains can break, offering a way to measure the attractive strength between two defects. During motion of a droplet, the changing birefringence, which differs parallel and antiparallel to the direction of motion offers a probe of the flow lines (fig. 1 (right)). Further, in the wake of the flow, a defect line is formed, which annihilates after droplet motion ceases. Pattern formation within the ferrofluid is expected to have a profound influence on the director field of the liquid crystal.

We have thus realized a hybrid system of a ferrofluid dispersed in a nematic liquid crystal. These multifunctional materials offer a wealth of potential in electrooptic, magnetooptic or sensor application, as well as elasticity and fluid dynamics of liquid crystals, via the interaction of a phase separated system, where one phase is magnetically and the other electrically responsive.

References

[1] S. Odenbach (ed.), Colloidal Magnetic Fluids, Springer, Berlin, (2010).

Polymer enhanced LCs with continuous optical phase modulation

A. Lorenz[a], L. Braun[b], V. Kolosova[b]

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[b] *Stranski-Laboratory, TU Berlin, Berlin, Germany*

Recent advances in polymer enhanced LCs are reported. Continuous optical phase modulation *[1]* with desirable electro-optic response properties was obtained by doping the common LC mixture E7 with 10% of a mixture of both non-mesogenic and mesogenic acrylates and a small amount of photoinitiator *[1]*. The doped LC was filled in LC test cells with planar ITO-electrodes and narrow (2 – 6 µm) cell gaps. The test cells were investigated by polarized optical microscopy. Upon photo-curing with a UV LED (Winger), the uniform director alignment inside the LC test cells was maintained. The voltage dependent transmission properties of the LC were investigated; the LC test cells were aligned in a temperature controlled sample holder, oriented in 45°-direction in-between crossed polarisers, electrically addressed with voltages in the range of 0-20 V and investigated (Figure 1) with both monochromatised light and white light, respectively.

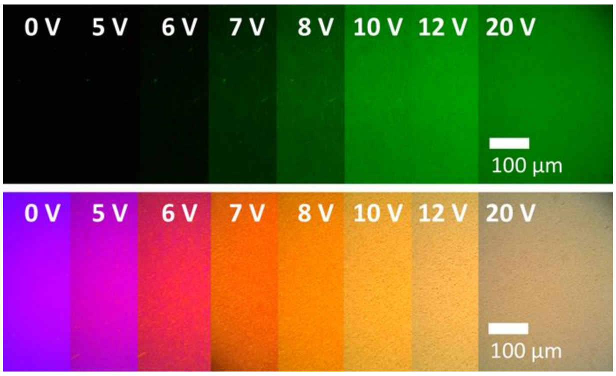

Figure 1. Micrographs recorded in a copolymer network nematic LC at different applied voltages with monochromatized light (green wavelength) and with white light, respectively.

In the first case, modulations of the transmittance were detected. In the second case, modulations of the characteristic Michel-Levy birefringence colors were induced. The electro-optic responses were carefully analyzed with a tilting compensator and a photo-multiplier tube module, respectively. The LC showed desirable electro-optic responses with sums of response times $t_{on}+t_{off}$ = 2.4 ms at moderate driving voltages < 20 V. A characteristic linear dependence of the response time t_{off} and addressing voltage was found. In conclusion, continuous phase modulation with phase modulation depth > 2π was found at driving voltages one order of magnitude lower than in chiral variants of the same or comparable host LCs *[2-4]*, and 2 – 3 times lower than in polymer network nematic LCs selectively stabilized with mesogenic monomers.

References

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[2] R. M. Hyman, A. Lorenz, T. D. Wilkinson, Liquid Crystals, 1-8 (2015). DOI: 10.1080/02678292.2015.1061146
[3] R. Hyman, A. Lorenz, S. M. Morris, T. D. Wilkinson, Applied Optics 53, 1 (2014).
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[6] J. Sun and S.-T. Wu, Journal of Polymer Science Part B: Polymer Physics 52, 183 (2014).

Proposing a generalized conservation law for main-chain polymer nematics

D.Svenšek[a], R. Podgornik[a,b,c]

[a] *Department of Physics, Faculty of Mathematics and Physics, University of Ljubljana, Slovenia*
[b] *Department of Theoretical Physics, "Jožef Stefan" Institute, Ljubljana, Slovenia*
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Liquid crystalline order is ubiquitous in biological materials and many properties of these systems can be analyzed in terms of the standard Landau-de Gennes approach, without particularly worrying about e.g. the polymer nature of the main-chain polymer nematogens. Nevertheless, it was recognized a while ago, that the Landau-de Gennes approach needs to be modified specifically to take into account the polymer nature, i.e. the microscopic connectivity of the underlying mesogens *[1,2]*. This connectivity leads to a coupling between the positional and orientational order of the polymer molecules. The ensuing "continuity equation" was shown to matter fundamentally for a consistent description of macroscopic properties of these systems *[3,4]*.

However, recently we showed that depending on the nature and the symmetry of the mesophase order, this continuity equation might not be the only condition that the mesoscale description of polymer nematics needs to satisfy. In fact, its generalised form in terms of a vectorial conservation law *[5,6]* suffices for polar nematic order, while in the more usual quadrupolar nematic order case a different, tensorial conservation law exists *[6]*. Discovering a new form of the conservation law naturally leads to the question, which form is the correct one, how are they related and when one should use one as opposed to the other one. In this contribution we address and resolve these fundamental questions. Among others, we show that flexible chains with strong backfolding, and thus with a vanishing local mesoscopic polar order of chain tangents, should satisfy the tensorial conservation *[7]*. Moreover, we elaborate on the correct application of both conservation laws to the general case of semi-flexible chains, which should include the limits of inflexible and flexible chains as special cases. Finally we show that the correct penalty potential in the free energy, implementing this generalised conservation law, should actually connect both the tensorial and the vectorial constraints. The consequences of the connectivity of the main-chain polymer nematics for their mesoscopic description are thus highly non-trivial.

$$\nabla \cdot (\rho\, \mathbf{a}) = 0$$

vs.

$$\partial_i \partial_j (\rho\, Q_{ij}) + \tfrac{1}{2} \nabla^2 \rho = 0$$

Figure 1. Vectorial and tensorial conservation laws in the absence of chain ends acting as sources.

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Liquid crystal technologies towards realising a field sequential colour (FSC) display

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In a conventional liquid crystal display the liquid crystal merely has the role of a ‘light shutter’. Application of different voltages to a liquid crystal element allows the amplitude of transmitted light to be accurately controlled. In order for colours to be realised colour filters have to be used. Even in the case of a white backlight that is formed using quantum dots, giving narrow spectrum red, green and blue, this still means that at least 66% of the light is absorbed by the colour filters.

When analysing the total efficiency of a liquid crystal display, high losses from the colour filters combine with losses from other layers to give a throughput from the backlight to the user of only 6-9%. This is something to consider next time the ‘low battery’ symbol appear on your smartphone, since the backlight uses in the region of 40-70% of the total power. The efficiency of a liquid crystal display could be greatly improved by changing from a white backlight to a time sequential red, green and blue backlight, so called field-sequential colour (FSC) *[1]*. Any image can then be generated by quickly cycling between the red, green and blue frames to give an overall image that would be observed by the end user, as shown in Figure 1.

A consequence of FSC driving is that an effect known as ‘colour break up’ can occur, observed as a blurring of different colours particularly on the edges of images *[2]*. In order to eliminate the appearance of colour break up then fast switching LC modes need to utilised, two such examples of these are Blue Phase (BP) and Uniform Lying Helix (ULH) *[3-5]*. Both BP and ULH are being actively investigated and both appear capable of providing the switching speeds that would be needed to realise a transmissive FSC display.

Figure 1. By splitting the red, green and blue channels of an image it is possible to then re-construct a full colour image by quickly cycling between these RGB frames.

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Rationalising dye alignment in liquid crystal hosts through a combined experimental and computational approach

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The optical properties of guest dyes dissolved in liquid crystal hosts mean that these systems can potentially be used in a wide variety of practical applications. Early proposals to use such systems in display devices have more recently been extended to a more diverse range of applications.

A number of properties must be concurrently optimised for guest-host systems to be of use practically, and it is therefore desirable to develop a detailed understanding of the behaviour of dyes dissolved in anisotropic hosts. Typically, optimisation of the colour and colour intensity, the optical anisotropy, the electrochemical stability and the photochemical stability of a guest-host system is essential for its practical use, with the most important properties being determined by the specific application in question.

Recently we have developed a computational method of predicting the optical anisotropy of guest-host systems, by combining molecular dynamics to simulate molecular alignment with time-dependent density functional theory to calculate transition dipole alignment *[1]*. These calculations do not rely on the input of experimental data, and the results may be compared directly with the results of experimental polarised UV-vis absorption measurements of aligned guest-host systems, enabling experimental trends in order parameters to be rationalised.

Further analysis of the computational results has highlighted potential limitations in the use of the common models applied when considering the alignment of dyes within guest-host systems. Careful consideration of the alignment axes of dye molecules along with the influence of their molecular flexibility (Figure 1) has provided further insights into the underlying causes of the variation observed experimentally in the order parameters of a set of anthraquinone dyes in a nematic host *[2]*.

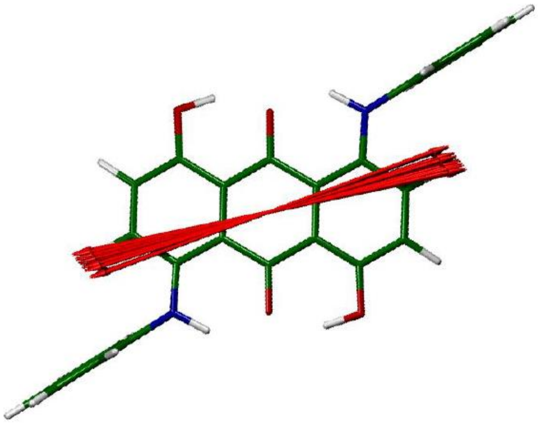

Figure 1. Influence of molecular flexibility of the transition dipole moment orientations of an anthraquinone dye.

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Liquid crystalline and spectroscopic properties of distorted arene cores

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Designing displays on flexible substrates with high energy conversion, brilliance, and chemical stability at low production costs are goals which require the investigation of new classes of organic semiconductors. Discotic and calamitic liquid crystals with semiconducting properties exhibit high potential to enhance the performance of organic electronics because of the self-organising properties of liquid crystals *[1]*.

In this study we focus on compounds with distorted arene cores, namely perylene esters (**1**) and *bay*-extended derivatives with either a phenanthroperylene- (**2**) or dinaphthocoronene-core (**3**) (Figure 1 (a)) *[2-4]*. It is revealed that the distorted cores induce columnar liquid crystalline mesophases, even if the compounds have relatively short side chains. At the same time the spectroscopic properties change unexpectedly with each extension of the core. Not only increases the absorption in the ultraviolet region, but also the fluorescent behavior changes.

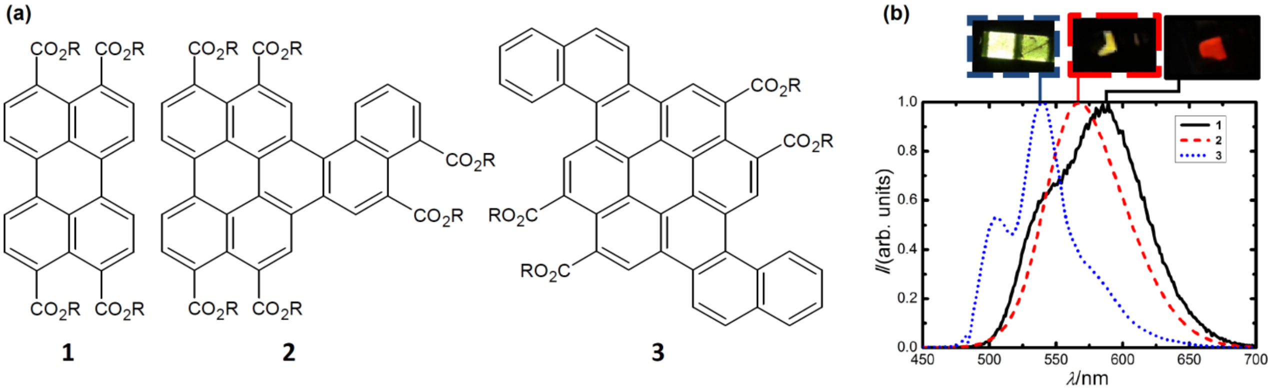

Figure 1. (a) Chemical structure of esters with a perylene- (**1**), phenanthro[1,2,3,4,*ghi*]perylene- (**2**), and dinaphtho[1,2-*a*:1',2'-*j*]coronene-core (**3**). (b) Electroluminescence spectra of compounds **1** – **3**.

Furthermore, the luminescent emission of the compounds in the solid state is influenced by the distortions, which is of significant importance for the application of these compounds as emitter materials in electroluminescent devices (Figure 1 (b)). These results were obtained by employing UV-Vis spectroscopy, fluorescent spectroscopy, x-ray diffraction (XRD), cyclic voltammetry and differential scanning calorimetry. Additionally, the experimental data is supported by calculations based on time-dependent density functional theory.

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Persistence length of chromonic aggregates

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Chromonic mesogens are non-conventional amphiphiles, which, in aqueous solution, self-assemble to form aggregate structures: rods, stacks or layers. These aggregates can subsequently self-assemble to form chromonic mesophases. Initial self-assembly is strikingly different to that seen in most conventional amphiphiles: typically being promoted by the interaction of aromatic ring systems and taking place in the absence of a critical micelle concentration. Once an equilibrium distribution of aggregates has been achieved, the proximity of aggregates, and hence concentration, can control the onset of ordered phases *[1]*.

Given chromonic aggregates form with an isodesmic (or close to isodesmic) association, the distribution of aggregate sizes is implicitly linked with the binding energy of any pair of molecules. Recent simulations *[2,3]* have calculated the binding energy of multiple chromonic systems and found chromonic molecules can have a large range of binding energies, but, this does not necessarily correlate with the onset concentration of the nematic phase.

In this presentation we address the inability to predict the onset concentration of the nematic phase from binding energy alone, and show how factors such as aggregate flexibility can have a critical impact on the nematic phase properties. Here we use metadynamic simulations to quantify the persistence length of chromonic aggregates for two sample systems, an ionic chromonic (sunset yellow) and a non-ionic chromonic (TP6EO2M).

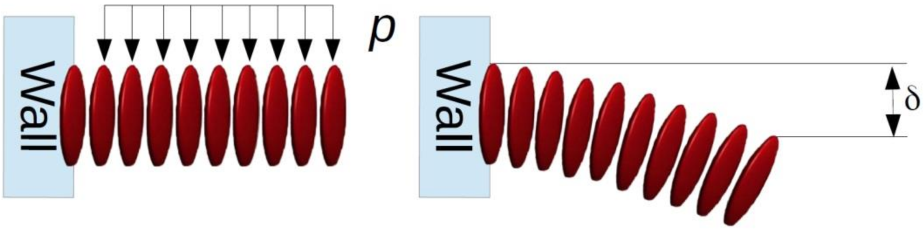

Figure 1. Schematic showing metadynamics simulation to calculate aggregate deflection with fixed load.

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Order parameters from ^{1}H NMR using the Haller extrapolation

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The temperature dependence of the nematic order parameter follows an empirical relationship known as the Haller equation *[1]*. This relationship has been widely used for obtaining order parameters from, e.g., birefringence, UV and IR absorption, Raman scattering, and dielectric permittivities. For these properties, the local electric field is usually not known and the reference value for perfect order must be obtained by extrapolation. On the other hand, for magnetic properties, that is, for diamagnetic susceptibilies as well as NMR interactions, the problem of the unknown local field does not exist and absolute order parameters can be determined. In particular, NMR spectroscopy has been proven to be a very powerful method for the detailed analysis of the molecular order in liquid crystals, cf. for instance, *[2]*. The validity of the Haller relationship for NMR data has been investigated as well *[3]*.

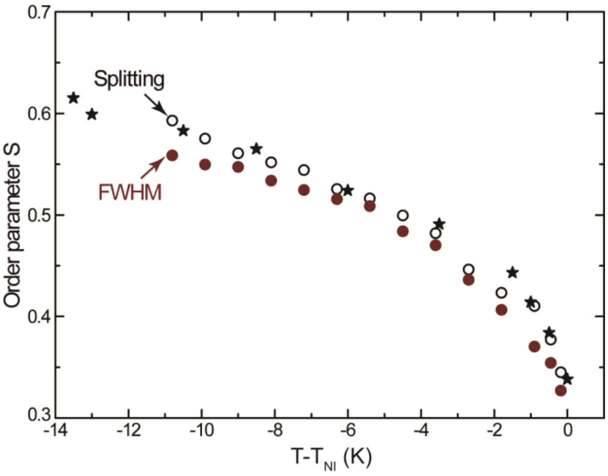

Figure 1. Order parameter of 5CB obtained from ^{1}H NMR spectra using the Haller extrapolation. For comparison, the data from ref. *[2]* are shown as stars.

Here, we suggest a simple procedure to estimate order parameters from one-dimensional ^{1}H NMR spectra of fully protonated liquid crystals by applying the Haller relationship to the temperature-dependent splitting of the dipolar doublet or the full spectral width at half maximum (FWHM) *[4]*. The method was applied to 5CB and E7 and found to yield order parameters in good agreement with previous reports *[2]*. As the method requires no isotopic labeling, no specialised instrumentation, and neither complicated NMR pulse programs nor model-based data analysis it allows us to estimate order parameters in an easy way and is potentially useful as a routine characterisation method for calamitic liquid crystals.

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Sensing potential: the use of chiral nematic thin films incorporating reactive chiral dopants as sensors

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Liquid crystalline sensors that utilise reactive chiral dopants are a growing area of interest, due to the ability of the nematic host to amplify small changes in the state of the dopant. Such sensors have been developed for a range of analytes, including water vapour *[1]*, CO_2 *[2]*, barbiturates *[3]* and acetone *[4]*. These work on the basis that a chemically induced change in the helical twisting power of the dopant results in a change of the wavelength of maximum reflection (λ_{max}).

In order to aid in the screening of potential reactive dopants for sensor materials, we have developed a model which aims to predict the change in λ_{max} for a given analyte concentration. From this, the potential sensitivity and dynamic range of a sensor can be calculated. I will present the results of the application of this model to our recent work on acetone sensors, as well as discuss limitations of these types of sensors, and ways to bypass these limitations.

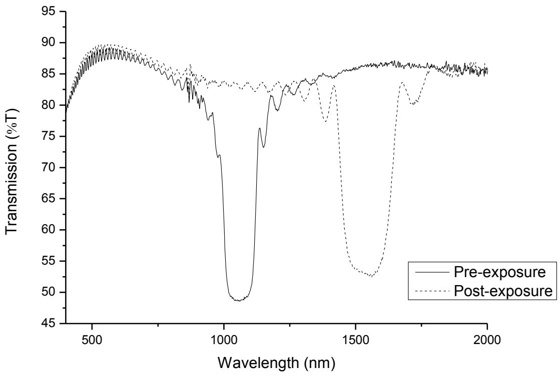

Figure 1. Change in λ_{max} before and after exposure to UV light.

These conclusions were also applied to our other work: I will present recent results on a new UV sensor, based on the UV-induced photoracemisation of a chiral dopant, which shows unprecedented sensitivity, with changes in λ_{max} of hundreds of nanometres. The potential of these sensors as a personal monitor of UV exposure will also be explored.

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Using absorption bands for photonic band gap engineering in cholesteric liquid crystals

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Due to their chiral molecular order, cholesteric liquid crystals (CLCs) act as one-dimensional photonic crystals. Conventional systems exhibit exactly one selective reflection band (SRB), i.e. one photonic band gap for circularly polarized light with the same helicity as the cholesteric order. In a theoretical treatment, we show that double reflection bands can be created by introducing narrow-band absorption into the liquid crystal.

The limiting vacuum wavelengths of the SRB are $n_o p$ and $n_e p$, where p is the cholesteric pitch and n_o, n_e are the ordinary and extraordinary refractive indices of the quasi-nematic planes, respectively. As dispersion and dissipation in an optical medium are linked by the Kramers-Kronig relations, an isolated absorption band ($n'' > 0$, Fig. 1a) is always accompanied by a wavelength interval $[\lambda_1, \lambda_2]$ of anomalous dispersion ($dn/d\lambda > 0$); for long wavelengths ($\lambda > \lambda_2$), the refractive index (n') is always larger than the refractive index for short wavelengths ($\lambda < \lambda_1$), cf. Fig. 1b. If the refractive index variation introduced by an absorption band is strong enough, the wavelength inside the medium shows a non-monotonic behaviour as a function of the corresponding vacuum wavelength; in case of an absorbing CLC, by choosing the cholesteric pitch appropriately, then the condition $n_o p < \lambda < n_e p$ for selective reflection is matched not only for one single wavelength interval, but for two wavelength intervals (Fig. 1c). Therefore, a strong and narrow absorption band can give rise to two selective reflection bands (Fig. 1d).

Possible applications of this effect include multi-colour reflectors and liquid crystal lasers (where the additional band edge resonances might allow for improved pumping schemes as well as for multiple-wavelength emission).

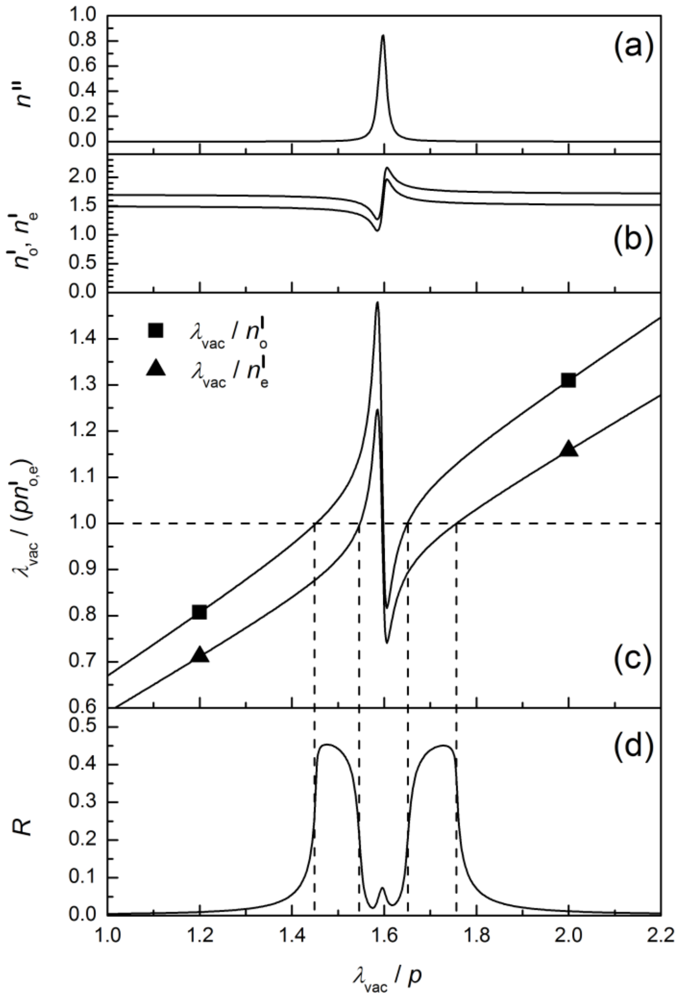

Fig. 1. Absorption band (*a*) and corresponding dispersion relations (*b*) in a CLC; wavelength intervals $\lambda_{vac}/p \in [n_o, n_e]$ (*c*, intervals are indicated by vertical dashed lines); resulting reflectance spectrum of a CLC (*d*; assuming unpolarised illumination and neglecting multiple reflections); the abscissa for all plots is vacuum wavelength (λ_{vac}) divided by cholesteric pitch (p).

Modelling of free-standing perovskite-chiral polymer film structures for lasing

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The distributed feedback presented by chiral nematic liquid crystals has made them attractive for lasing, particularly as a laser dye can be easily incorporated *[1]*. However, these devices are limited by the laser dyes, which have chemical and photo-instabilities amongst other issues *[2,3]*. Perovskite has been demonstrated to be highly luminescent, and could replace laser dyes as a gain medium *[4,5]*. A device is proposed for lasing: a thin layer of perovskite between chiral polymer films. Characterisation and modelling of the device are presented.

Two possible structures are considered for this device, shown in figure 1. For the stack structure (fig. 1(a)), each layer is spin coated on top of the previous layer. For the sandwich structure (fig 1(b)), the polymer films and perovskite are spin coated onto glass, with the perovskite then placed between the films.

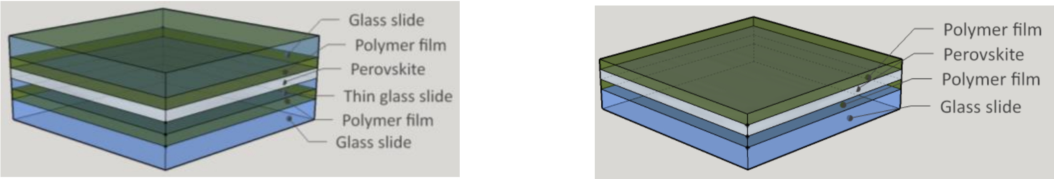

Figure 1. The (a) stack and (b) sandwich structures for a perovskite-polymer film device.

The stack structure has been fabricated, and the band edge of the chiral polymer films coincides with the emission from the perovskite. The emission wavelength can be chosen at the point of perovskite fabrication, and so a range of wavelengths are possible, and can be matched to the chiral film bandgap. The fabrication of the polymer films has been to shown to be key in producing good devices. The photonic bandgap of these films is strongly dependent on the curing conditions. Characterisation of these devices through polarising optical microscopy and spectral analysis indicates potential for moving towards lasing emission.

To model aspects of lasing in these devices, the Berreman 4×4 matrix method is used *[6]*. Gain is introduced by means of an imaginary component of the refractive index of the perovskite. The modelling results highlight the importance of the thicknesses of the perovskite and polymer film layers, which provide gain and optical feedback respectively. Reflection from the optical cavity formed by the perovskite interfaces is shown to interfere with the polymer film stopband, and the thickness can be varied to alter the reflection profile, which itself would impact lasing. Balancing this with an appropriate thickness for gain, and practical limitations of fabrication, will be crucial in achieving lasing in these structures.

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Poiseuille flow of cholesteric liquid crystals

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The flow response in cholesterics is strongly non-Newtonian, highly anisotropic and complex. Theoretical studies showed that a standard cholesteric phase subjected to Poiseuille flow along its helical axis flows mainly through permeation at small pressure differences, leading to high dissipation and very large viscosities *[1]*. If the helix is oriented along the vorticity direction travelling twist waves appear which cause a rotation of the cholesteric helix. Under higher forcing, the helix uncoils, creating a flow-induced nematic phase *[2]*.

Most of these pioneering results have been derived under specific assumptions like the absence of defects or the constraint that the molecules may only rotate in the flow-gradient plane whilst the orientation of the cholesteric helix remains unchanged. Building on our expertise in large-scale simulation of liquid crystals we are able to investigate more general situations. We present new results on the flow of cholesteric fingers and blue phases in microfluidic channels. Depending on the pressure gradient between inlet and outlet, the geometry and anchoring conditions at the channel walls we are able to characterise different flow regimes. These results add to the picture that we previously gained from cubic blue phases in simple shear flow *[3]*.

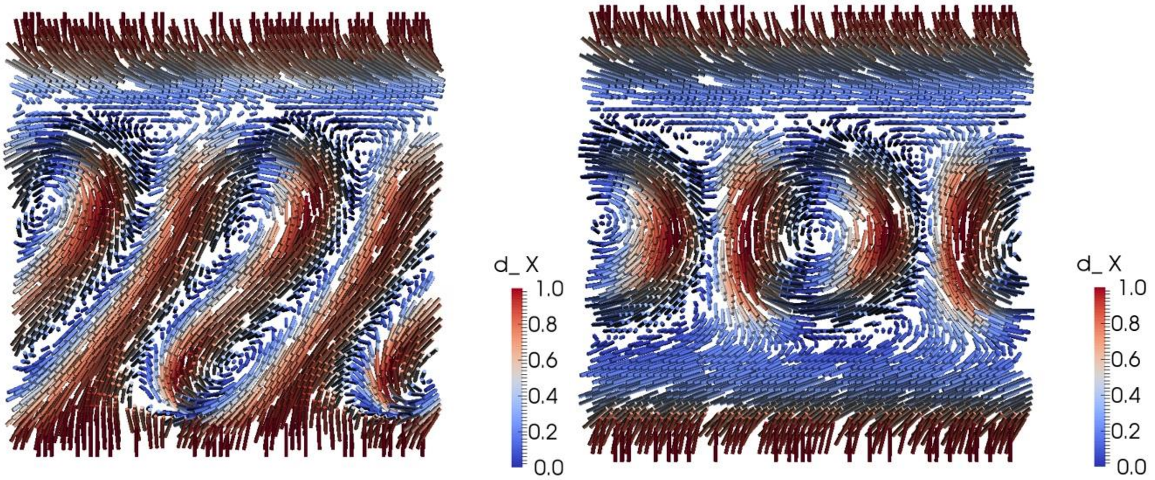

Figure 1. Cholesteric fingers of the first kind (CF-1) in Poiseuille flow for different pressure gradients between inlet and outlet with normal anchoring at the top and bottom walls.

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Liquid crystalline actuating Janus-particles by a co-flow microfluidic synthesis

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Liquid crystalline elastomers (LCEs) have been used as suitable materials for actuator applications, such as stimuli responsive actuating microparticles *[1-3]*, thin films, fibres or artificial cilia. LCEs are slightly crosslinked liquid crystalline polymers which exhibit a macroscopic shape transformation during the phase transition of the liquid crystalline and the isotropic state. This stimuli responsive shape transformation is completely reversible and depends on the geometry of the LCE's director field. A capillary based microfluidic set-up *[4]* enables the formation of microdroplets as well as a systematic orientation of polymerisable mesogens by shearing dispersed droplets in a highly viscous continuous flowing silicone oil. Further UV-induced polymerisation and crosslinking of the LC-monomer droplets in the nematic phase leads to actuating LCE-particles.

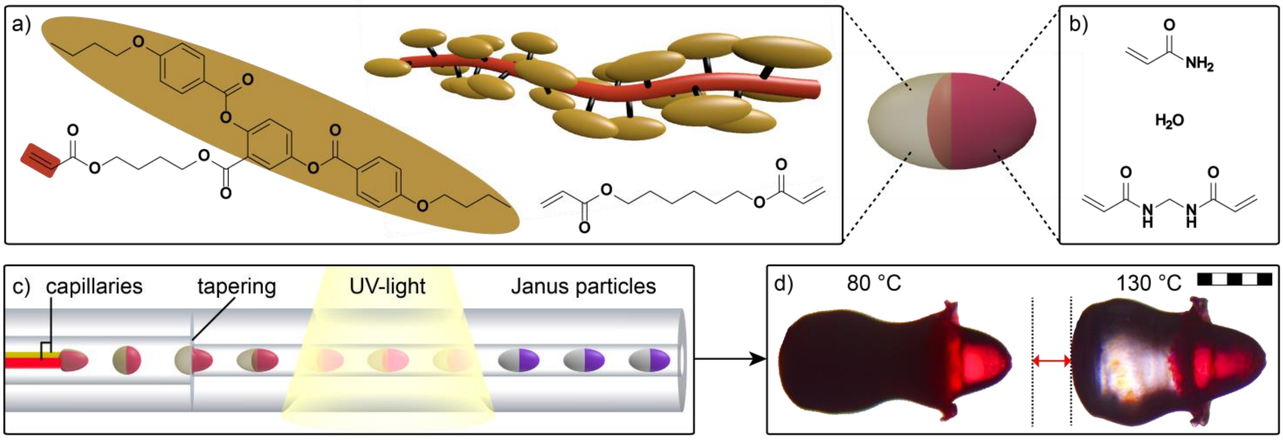

Figure 1. Compounds of the Janus particle's a) liquid crystalline and b) hydrophilic part; c) Capillary based microfluidic Janus-droplet formation and polymerisation; d) Thermal actuation of a Janus-particle

In this work the microfluidic synthesis and characterisation of Janus-particles, consisting of an actuating hydrophobic LCE-part and a non-actuating aqueous hydrophilic part, is presented. Two capillaries provide the phase separating monomer mixtures (Fig. 1a, 1b), forming Janus droplets which are strongly sheared by tapering the polymerisation tube (Fig. 1c). The resultant elongated Janus-particles exhibit a bipolaric director field *[3]* which leads to a contracting actuation along the particle's rotational axis, observed by heating the particles above the LCE's clearing temperature (Fig. 1d). The Janus-particle's size, morphology and actuation properties were controlled by varying the parameters of the microfluidic set-up and further studied by POM and WAXS measurements.

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Dynamics of defects in shells of active liquid crystal

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We propose a hydrodynamic model for a thin spherical shell of active nematic liquid crystal with fast elastic reorientation. Active flows are driven primarily by topologically required defects in the alignment, for which we derive exact expressions within the thin film approximation. When active flows dominate the defect dynamics over elasticity they lead to an attraction between defects of the same topological charge. For four +1/2 charge defects we find in simulations different regimes of periodic motion depending on the ratio of activity to elasticity: oscillations between tetrahedral and planar configurations, as seen in experiment *[1]*, and activity-driven separation into pairs forming +1-defect-like structures (see Figure 1). In the purely hydrodynamic regime we observe the coalescence of two +1 charge defects into Boojum textures. The tangential part of the flow has stagnation points with integer strength windings, which has strong implications for the three-dimensional nature of the flow.

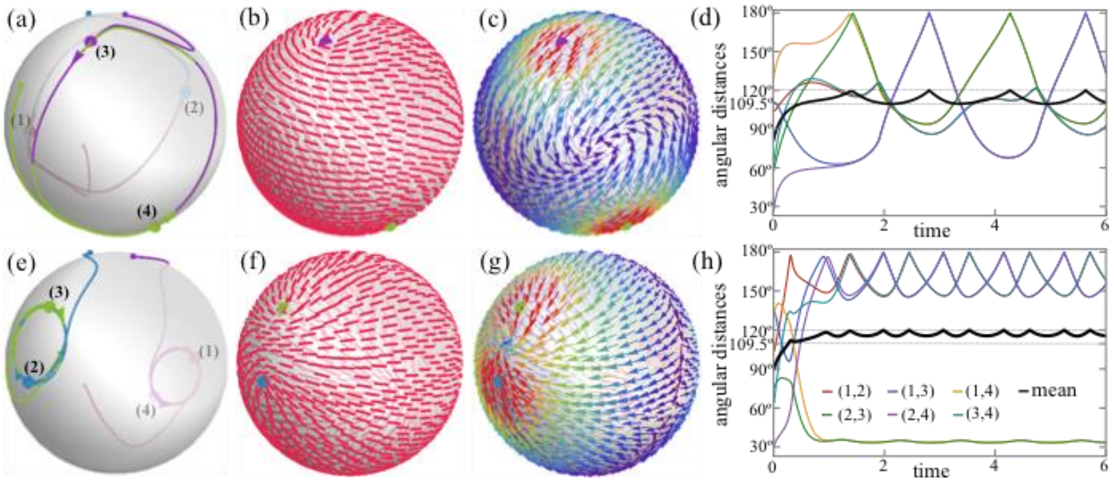

Figure 1. (a)-(d): Elasticity dominated regime with oscillations between (skewed) tetrahedral (b) and planar configurations. (e)-(h): Active hydrodynamics dominated regime, where defects separate into pairs with ellipsoid orbits and effectively form two +1 defects. Each row shows (from left to right): trajectories of four +1/2 defects starting at random positions, orientation field and flow field for positions marked in trajectories, and pairwise and mean angular distances over time, where (i, j) denotes distance between defects marked as (i) and (j) in trajectories.

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Virtual polarising microscopy on nematic shells

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Liquid crystals confined in shell geometry have evolved into a hot topic of soft matter research due to their potential for intriguing applications *[1]* and great opportunities for studying defects *[2]*, which are inevitably formed due to topological constraints. In our current study, we utilise numerical simulations for a deeper analysis of polarising optical microscopy (POM) textures and the formation of topological defects in nematic shells.

We simulate the director configuration within the shells by using an established tensor approach for minimising the total free energy F_{total} of the liquid crystal *[3]*. Virtual POM textures are obtained by calculating the light propagation through the shells via Jones calculus. The resulting textures are compared to experimentally observed POM textures of 5CB shells produced in a coaxial glass capillary microfluidic set-up *[4]*.

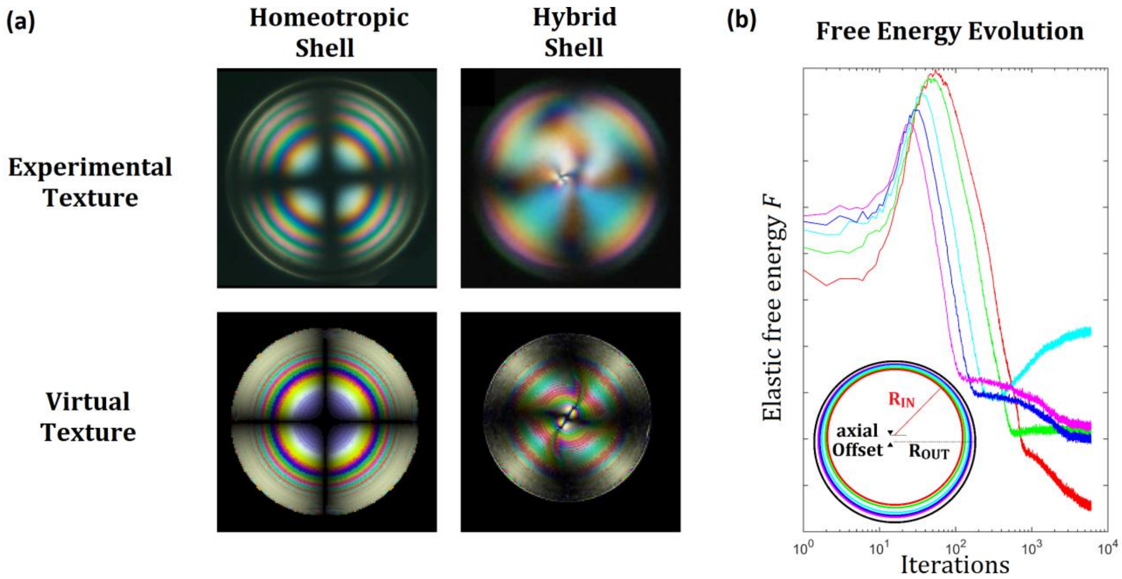

Figure 1. (a) Exemplary experimentally observed polarising microscopy images (top) and simulated textures (bottom) for shells with homeotropic and hybrid alignment, respectively. (b) Evolution of the elastic free energy during the director field relaxation for simulated shells with hybrid alignment and varying ratios of inner to outer radius.

We show that our simulation approach is capable of reproducing experimentally observed textures with respect to colour and defect location (cf. Figure 1 (a)). In contrast to the experimental situation, we can simulate virtual textures for arbitrary observation directions, which is challenging to achieve in a laboratory experiment. The evolution of elastic free energy is screened during the director relaxation process, which offers a deeper understanding of the defect formation in shells of varying size ratios between inner and outer radius or differing axial offset (cf. Figure 1 (b)). The latter parameters are easily adjusted in our virtual model, which allows us to analyse in detail the formation of two +1 defects and their relative position within hybrid shells.

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Mesophase behaviour in dimeric systems with a nematic-nematic transition

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Nematics are the simplest and the most widely studied liquid crystalline systems. The recent discovery of a new nematic phase *[1,2]*, initially reported in certain types of symmetric liquid crystalline dimers with odd carbon-number alkyl spacers, is receiving increasing attention [3-5]. This low temperature nematic phase termed Nx, which is chiral in nature even though comprised by achiral molecules, poses new challenges in the research field of liquid crystals, as the correlation of the mesomorphic behaviour and physicochemical properties of the Nx with the molecular features and self-assembly of the constituent molecules is not yet well understood.

Within this framework we make a contribution to the understanding of this phase by investigating the mesophase behaviour of new dimeric systems, with lateral and terminal dipoles, and mixtures, in order to investigate the least molecular parameters responsible for the formation of the phase and the stability of it in mixtures. Complimentary characterisation techniques, such as Polarising Optical Microscopy (POM), Differential Scanning Calorimetry (DSC) and X-ray Diffraction (XRD) are implemented in order to probe the physical and structural properties of the mesophase. The results are presented, while structure-property relationships and their impact on the Nx phase formation are discussed.

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Mirror symmetry breaking in cubic and isotropic liquid phases of achiral polycatenar molecules

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Chirality synchronisation of achiral molecules into macroscopic chiral superstructures is an emerging field in liquid crystal research *[1]*. Especially the formation of spontaneously chiral bicontinuous cubic phases, like *I*432 *[2]* and chiral isotropic liquids *[3]* represent a new field to explore.

Herein we report a new homologous series of polycatenar compounds based on 5,5´-diphenyl-2,2´-bithiophene. These compounds were synthesised and characterised by polarizing microscopy, differential scanning calorimetry and XRD (Figure 1). Depending on the chain length (n = 2−18) smectic, nematic and two distinct types of bicontinuous cubic phases were observed, one with *Ia*3;¯*d* and the other with *I*432 space group. Compounds with n = 2,4 form smectic and nematic phases, whereas all other compounds show bicontinuous cubic phases with *Ia*3;¯*d* and *I*432 lattice. The *Ia*3*d* phases are achiral, whereas a conglomerate of chiral domains is found for the *I*432 phases. As a special feature a reversible temperature dependent inversion of chirality was observed within the temperature range of the bicontinuous cubic *I*432 phases of some of the homologues. In addition chiral isotropic liquids, composed of a conglomerates of chiral domains (Iso* phases), appears above the cubic phases of most compounds, independent on the cubic phase symmetry. The width of the Iso* phases is strongly chain length dependent.

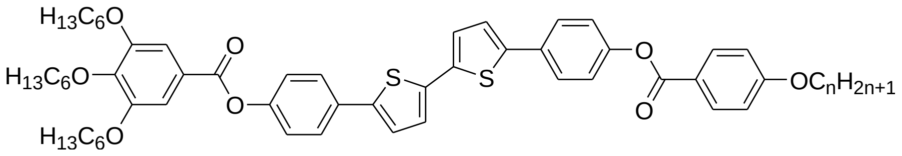

Figure 1: Structure of discussed tetracatenare liquid crystals (n = 2-18)

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Atomistic simulation of liquid crystals: towards the accurate prediction of phases and phase transition temperatures

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We present GAFF-LCFF, an improved atomistic simulation force field for the study of liquid crystals. The new force field has been tuned to reproduce the densities and heats of vaporisation of a series of liquid crystal fragments with high accuracy. The tuning work, uses a series of high-accuracy quantum chemical calculations for intramolecular interactions, and small molecule molecular dynamics calculations for intermolecular interactions.

We show that most earlier force fields misrepresented the flexibility of liquid crystal molecules, leading to many erroneous predictions for order parameters, densities and clearing points. We illustrate the success of the new force field through reproducing clearing points for a series of liquid crystals.

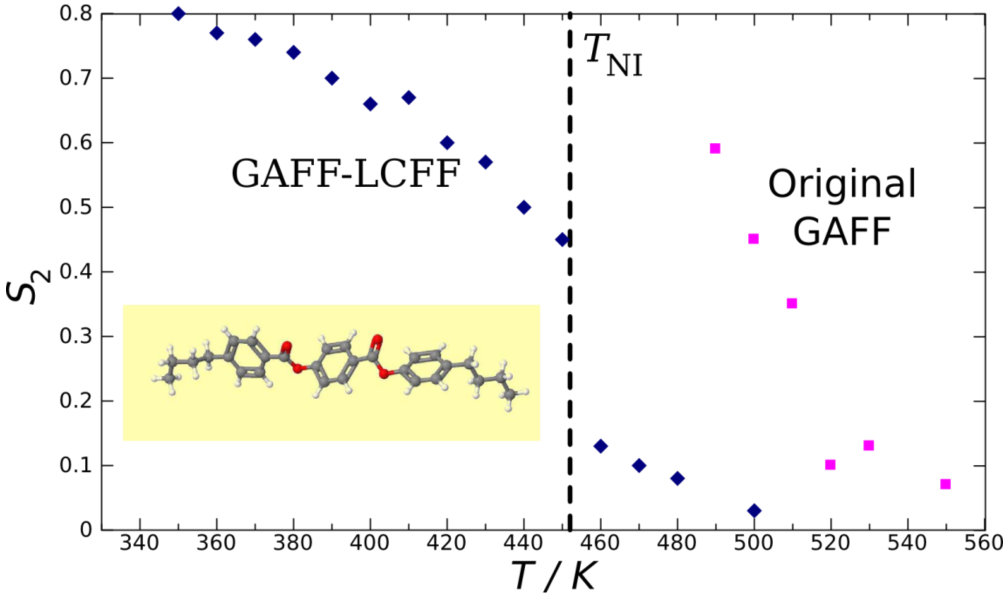

Figure 1. Performance of the GAFF-LCFF force field for the nematogen 1,3-benzenedicarboxylic acid,1,3-bis(4-butylphenyl)ester (an “exact” prediction for the clearing point is given, which is an improvement of 60 °C over the original GAFF force field).

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Retarded rupture of LC shells and bubbles in viscous environment

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Liquid crystalline shells in aqueous environment are interesting model systems, e.g. for studying director arrangements under variable anchoring conditions or phase transitions in confinement. Sub-millimeter sized liquid crystal shells are typically produced using a microfluidic co-flow technique, and their size and film thickness may be varied by osmosis between unequal inner and outer fluids *[1]*. Most investigations were carried out in the nematic phase, whereas only little attention was devoted to the smectic phases so far. All these studies dealt with slow shape dynamics of the shells. Here, we are interested in the dynamics of bursting LC shells and bubbles in the nematic and smectic A phases, surrounded by an aqueous surfactant solution.

Rupture of thin fluid sheets is a widespread phenomenon in nature and technology, related to aerosol production or the stability of foams and emulsions. Such rupture processes usually occur on the time scale of milliseconds, and the disintegration of soap films is but one example. Under ambient conditions, the retraction of films of Newtonian fluids proceeds at constant velocity determined by momentum conservation *[2]*. A similar behaviour was found for rupturing sessile bubbles of 8CB in the smectic A phase in air, despite the layered structure of the film *[3]*.

The LC shells and bubbles in aqueous environment presented here strongly deviate from this behaviour: We find an immense slowing-down of the rupture velocity by about three orders of magnitude, particularly in the smectic phase (see Fig. 1). We present an experimental characterisation, an intuitive explanation and a novel hydrodynamic model approach for this phenomenon, based on both the viscosity of the surrounding fluid and the viscosity and structure of the films.

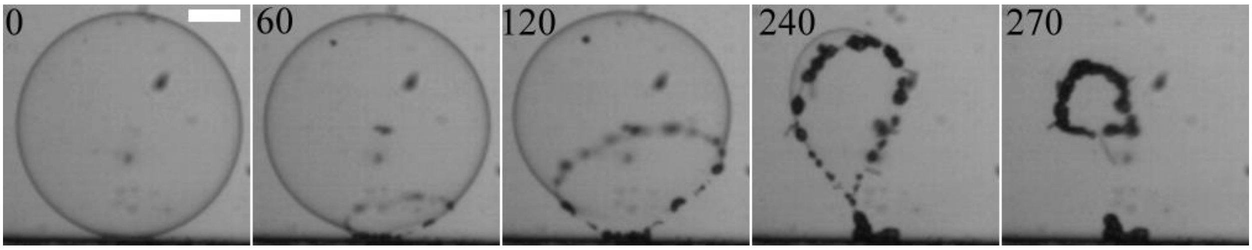

Figure 1: One of the observed rupture scenarios of smectic A shells filled with a glycerol/water mixture, submerged in water. Bar width: 50 µm, numbers: time after puncture in ms.

Work supported by DFG within grant STA 425/28.

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Multiscale models of freely rotating inclusions in nematic liquid crystals

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Suspension of nanoparticles in liquid crystals have been modelled on a range of scales, from molecular simulations to macroscopic models. The former are computationally expensive and only a few particles can be modelled. The second rely on macroscopic parameters whose values are not determined self-consistently.

In previous work *[1]* we have derived equations governing a nematic liquid crystal hosting fixed metallic inclusions with weak anchoring conditions. We used homogenisation theory *[2]* to obtain macroscopic governing equations containing effective material parameters that are related to the microscopic geometry by a series of cell problems. These describe the local effect of a single nanoparticle on the liquid crystal alignment and electric field based on the assumption that the nanoparticles are evenly distributed. The macroscopic equations for the director alignment contain three key differences with respect to those for a pure liquid crystal: (i) the elastic constants are in general smaller, (ii) there is a forcing term proportional to the anisotropy of the particles and, (iii) the dielectric susceptibility of the system is altered due to the fringe fields created by the particles.

Here we present the extension of this work to systems with freely rotating particles. The macroscopic equations describe how the particles influence the time dynamics of the liquid crystal in terms of parameters that depend only on the microscopic interaction between the two. In particular, depending on the strength of the particle-liquid crystal interaction the system may display one or two time scales.

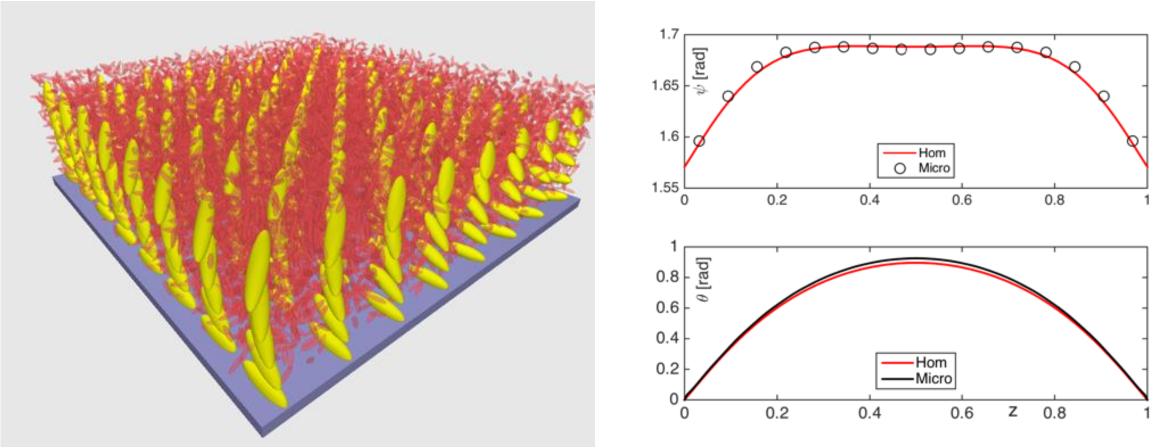

Figure 1. Left – Schematic drawing of the particles (yellow) immersed in a nematic liquid crystal (red). The orientation of the particles changes with position and time. Right – Comparison between macroscopic (red) and microscopic (black) equations for a one dimensional planar cell containing 16 particles. The top and bottom plots display the particle and director field angles respectively as a function of the position in the cell normalised to unit.

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Alignment and electro-optic properties of ferroelectric smectic C* liquid crystals with a direct transition to the nematic and isotropic phases

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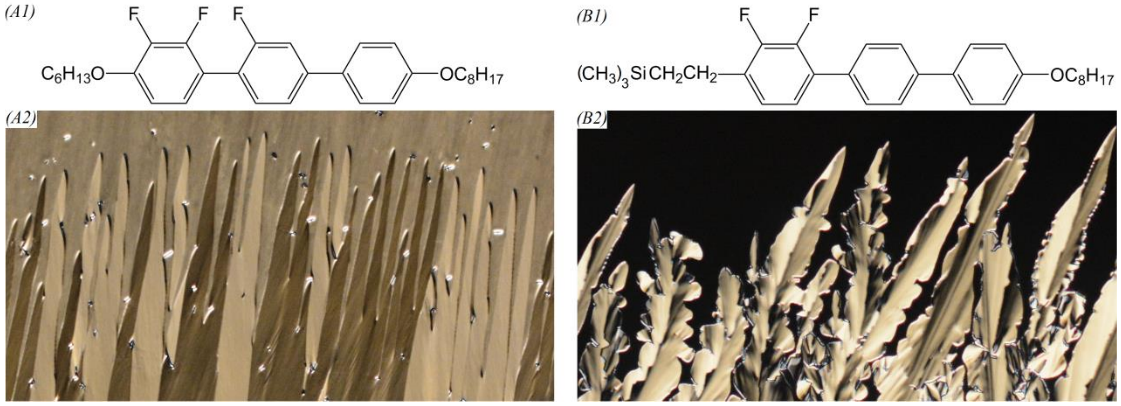
Ferroelectric liquid crystals have potential as fast electro-optic modulators and optical switches. Our aim is to design novel optical phase modulation with microsecond response times for use in telecommunication applications. These devices require temperature independent SmC* cone angles and uniform layer alignment. To obtain this, we investigate compounds with direct N- SmC and I-SmC phase sequences, and control the width of the nematic temperature range through mixtures of the compounds. We investigate the electro-optic properties of MH1079 (SmC-N-I) by adding a chiral dopant (BE80F2N*). Minimum dopant is added (0.5 wt. %) to avoid the introduction of a SmA phase. This provides the liquid crystal with a small ferroelectric spontaneous polarisation without alignment issues associated with chirality. Switching of the director about the layer normal is done by applying a polar electric field to the ferroelectric SmC* material. Extinction angle measurements are observed on a polarising light microscope. From this, and from the discontinuous phase transition between the SmC* and N* states, we find a high cone angle, though it exhibits some temperature dependence. When placed in a parallel rubbed cell, the nature of the phase transition results in a planar chevron structure, with the layer normal pointing at an angle of 20 degrees from the rubbing direction. The director of the SmC* phase is parallel to the rubbing direction without an electric field applied.

In an attempt to increase the cone angle silane end-group compound, EC10 that exhibits a direct SmC-I phase sequence, was added at various concentrations, each with 0.5 wt. % of BE80F2N*. The aim of this is to achieve a narrow N* phase to provide a means for good alignment of the SmC* molecules and achieve a temperature independent cone angle of 45 degrees. This has numerous applications in novel electro-optic devices and ultrafast liquid crystal phase modulators.



(A1) chemical structure of MH1079, (A2) N-SmC transition of MH1079, (B1) chemical structure of EC10 and (B2) I-SmC transition of EC10. The photographs were taken without applied electric field.

Electroclinic effect in a chiral lyotropic lamellar phase

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In thermotropic chiral smectic A (SmA*) phases, an electric field **E** along the smectic layers breaks the D_∞ symmetry of the SmA* phase and induces an inclination $\delta\theta$ of its director **n** with respect to the smectic layer normal **k**. This so-called *electroclinic effect* was first reported by Garoff and Meyer in 1977 and attracted substantial scientific and technological interest due to its linear and sub-microsecond electro-optic response *[1]*. While the electroclinic susceptibility, i.e. the electroclinic coefficient $(\partial\theta/\partial E)$, is rather low at higher temperatures, it diverges as the temperature is lowered towards the critical temperature of a second-order transition from the SmA* phase into the tilted ferroelectric smectic C* phase (SmC*) phase. With our recent discovery of the lyotropic analogue to the thermotropic ferroelectric SmC* phase *[2]* the question emerges, whether or not an electroclinic effect might also be observed in the chiral lamellar α (L_α*) phase close to its transition into the tilted and polar $L_{\alpha'}$* phase?

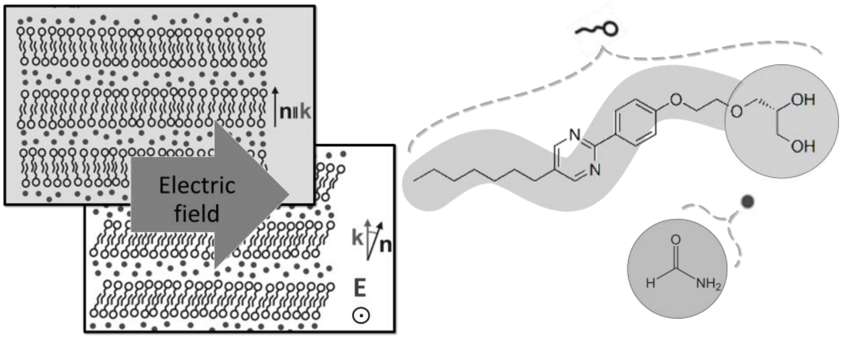

Figure 1. Electroclinic effect in a chiral lyotropic L_α* phase. On application of an electric field **E** the director **n** becomes tilted with respect to the layer normal **k**. The L_α* bilayers consist of chiral amphiphile molecules with 2-phenyl-pyrimidine cores and hydrophilic diol head groups; successive bilayers are separated by solvent layers (formamide).

Following the symmetry arguments of Garoff and Meyer *[1]* the electroclinic effect should exist in the lyotropic L_α* as well as in the thermotropic SmA* phases. However, in the lyotropic case the magnitude of the effect might be very small and, in addition, its experimental observation might be considerably complicated by the presence of the solvent, namely water or formamide, the electrolytic conductivity of which prevents the application of a (static) electric field. In this contribution we now report recent electro-optic experiments, which indeed led to the first observation of an electroclinic effect in the lyotropic L_α* phase. This effect is in many aspects found to be very similar to its thermotropic counterpart: the electroclinic response increases linearly with E and diverges as $(T - T_c)^{-1}$ when the temperature T approaches the transition temperature T_c into the tilted and polar $L_{\alpha'}$* phase. In the lyotropic case however the electroclinic response is strongly superimposed by the formation of electrolytic double layers, which screen the external electric field inside the lyotropic liquid crystal.

Financial support from the *Deutsche Forschungsgemeinschaft* is gratefully acknowledged.

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Probing lyotropic liquid crystal phases by a combination of EPR spectroscopy and molecular dynamics simulation

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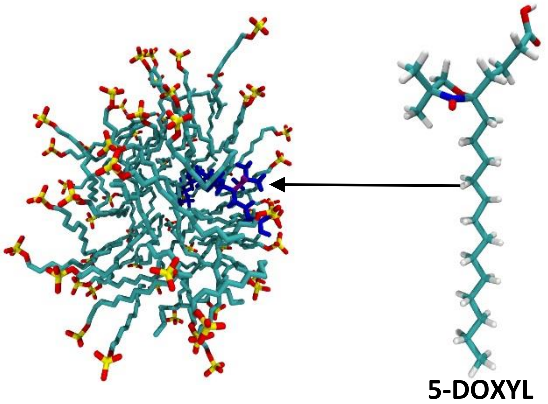
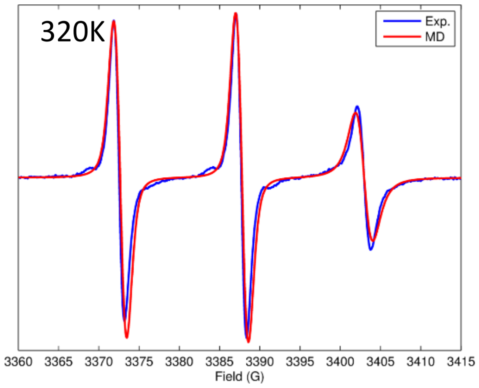
Electron paramagnetic resonance (EPR) is a ‘fast’ spectroscopic technique able to resolve the dynamics and molecular order of liquid crystal systems at the sub nanosecond timescale. However EPR spectral line shapes require thorough modelling and simulation to interpret spectra quantitatively. Here we expand our novel molecular dynamics-EPR methodology, previously used to study nematic and discotic thermotropic liquid crystals *[1-4]*, to sodium dodecyl sulphate (SDS) and dodecyltrimethylammonium chloride (DTAC) lyotropic liquid crystal aggregates doped with the 5-DOXYL stearic acid paramagnetic spin probe. Molecular dynamics trajectories generated using the General AMBER Force Field (GAFF) are used to directly predict EPR spectra *[1,5,6]* of pre-micellar, micellar and rod aggregates with the resulting line shapes showing good agreement with experiment. The simulations confirm the axial nature of the probe rotation in micellar and rod aggregates and allow this to be related to the rotational dynamics of the host liquid crystal molecules. Additionally, geometric parameters such as aggregate radii and area per molecule are found to be in good agreement with previous experimental studies.



5-DOXYL spin probe



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Orientational distribution functions and order parameters in “de Vries”-type smectics – a simulation study

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The detailed structure of “de Vries”-type smectic A (SmA) phases is still a subject of debate and often explained by the classical hollow cone model where all molecules have the same magnitude of tilt while the directions of tilt are randomly distributed *[1]*. More recent studies however suggest that the properties of “de Vries”-type SmA phases are also in-line with a conventional but very broad Maier-Saupe distribution function *[2]*.

We now simulated smectic A phases of rod-like particles with prescribed orientational distribution functions (ODFs), namely Maier-Saupe, diffuse cone and hollow cone distributions with same orientational order parameters S_2 and perfect translational order. For all simulated phases we calculated the corresponding 2D diffraction patterns by Fourier transform and analysed the diffuse scattering intensity related to the intra-layer correlations of the molecules (Fig. 1). We found that all three ODFs can be indeed distinguished by their 2D diffraction patterns, *i.e.* by the directional distribution of the diffuse wide-angle scattering. The comparison with experimental X-ray diffraction patterns indicate that the structure of “de Vries”-type SmA phases is better described by a Maier-Saupe ODF than by a hollow cone distribution.

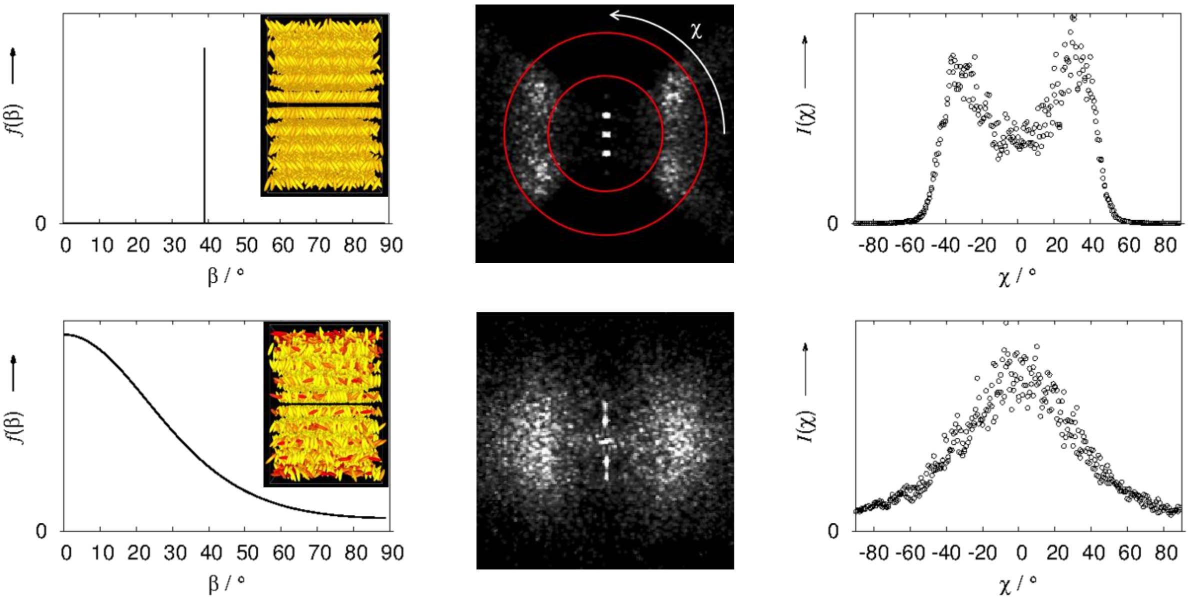

Figure 1. Top row: Hollow-Cone distribution (S_2 = 0.4). Bottom row: Maier-Saupe distribution (S_2 = 0.4). Left: Simulation snapshot of a smectic A phase of rod-like molecules with prescribed orientational distribution function *f*(β). β is the angle between the long-axis of a molecule and the liquid crystal director. Middle: Calculated diffraction pattern of the simulated phases depicted on the left. Right: Integrated profile of the scattering intensity between the red circles depicted in the middle.

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Self-assembled molecular wires of discotic liquid crystal formed with the crucial contribution of solvents

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Discotic liquid crystals can form columns along which charges flow. In a cell the LC typically assume homeotropic alignments with columns bridging opposite substrates, configuration attractive for solar cell applications while for other applications like sensors the in-plane orientation of the columns is preferred.

The self-organisation of discotic liquid crystal molecules allows the spontaneous formation of well-aligned and tens of micrometer long molecular wires as visible in the Figure below. In this work, we present a study based on hexapentyloxytriphenylene (HAT5) to investigate the molecular wire formation mechanism induced by solvents with selected characteristics, including chemical structure, boiling point, vapour pressure, and surface tension. The aromaticity in solvents such as toluene and benzene promotes the assembly into very long and thin wires entering into the structures, while chain-like solvents promotes more disordered structures. This finding allows a guided formation of different nanostructures from the same type of molecules just by choosing the type of solvent according to the need. Highly aligned molecular wires bridging electrodes on SiO_2 substrate show a clearly higher electrical conductivity compared to disorganized aggregates and bare HAT5. Raman spectroscopy, force microscopy, DLS and X-ray scattering were also used to investigate films and solutions. We finally discuss possible mechanisms behind the hierarchical assembly of the nanowires.

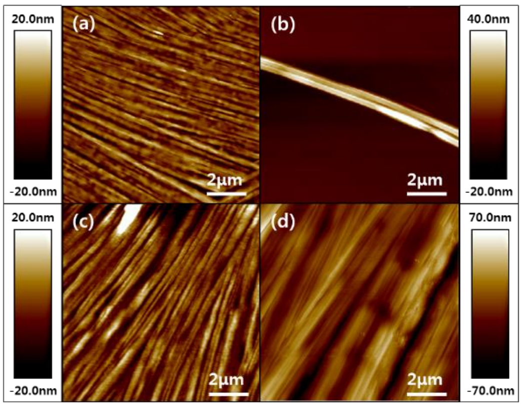

Figure 1. HAT5 deposited on substrate with different methods.

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O26

New shape-amphiphiles self-assembling in filled columnar mesophases

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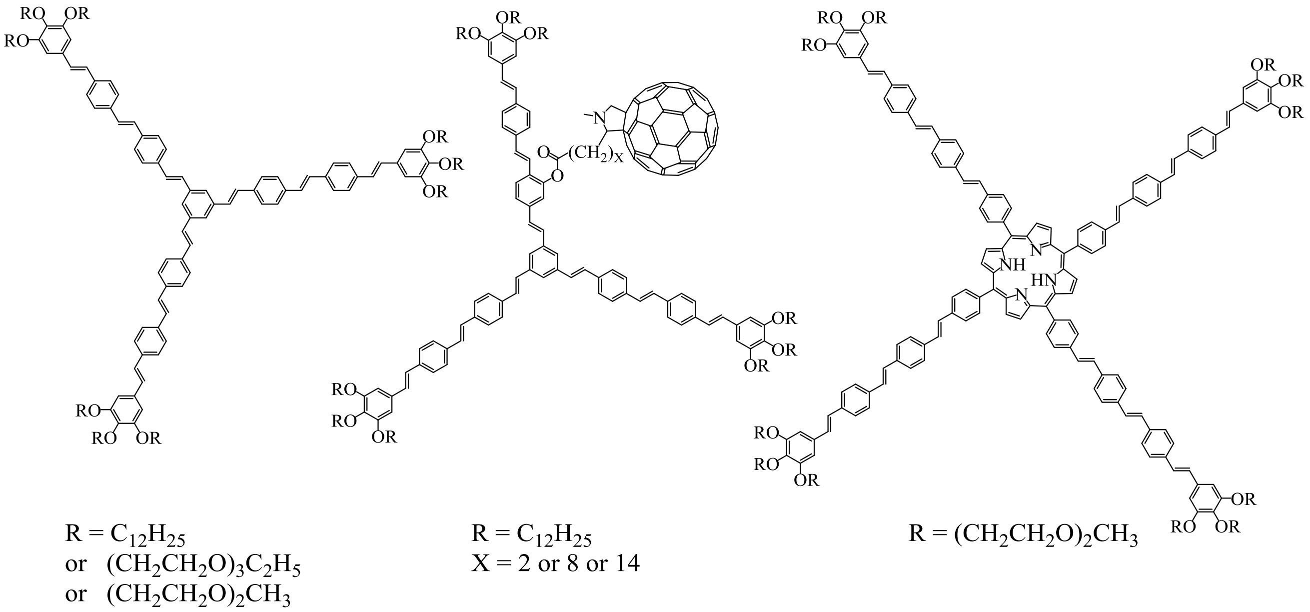
The driving force for the formation of most liquid crystalline phases is the nanosegregation of chemically or physically incompatible molecular building blocks. Conventionally they consist of rod- or disc-shaped rigid cores and peripheral aliphatic chains. The incompatibility can be produced also by different shapes like the combination of rods with discs or V-shaped molecules with rods [*1,2*].

In this contribution the design of star mesogens with oligo(*p*-phenylenevinylene) arms *[3]*, comprising intrinsic cavities in the core part, and their combination with spherical particles is highlighted (see figure 1). In these rigid molecules, the packing and nanosegregation of aromatic and aliphatic parts is possible by helical assembly and lateral translational displacement of the molecular centres from the columnar axis. The filling of this mesophase by incorporation of fullerene guests, covalently bonded via a spacer of various length, yields shape-amphiphiles, which self-organise in helical stacks of increased stability (T_{iso} > 280°C) *[4]*. The exchange of the peripheral alkoxy by oligoethyleneoxy chains revealed mesophases of much lower clearing temperatures, which is desirable for future photovoltaic applications. However, in some cases other than the expected LC self-assemblies have been discovered.

The synthesis of these compounds as well as their thermotropic properties and structures will be discussed, which were investigated by means of polarised optical microscopy, X-ray scattering, modelling and fibre diffraction simulation.



R = $C_{12}H_{25}$
or $(CH_2CH_2O)_3C_2H_5$
or $(CH_2CH_2O)_2CH_3$

R = $C_{12}H_{25}$
X = 2 or 8 or 14

R = $(CH_2CH_2O)_2CH_3$

Figure 1. Examined star-shaped compounds.

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Bent-core dimers utilizing benzenetriol central cores

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Bent-core liquid crystals have attracted considerable interest due to their unique properties, spontaneous polar order and macroscopic chirality of mesophases *[1]*. Several structural modifications which affect their mesomorphic properties have been investigated. Among others, dimerisation of various mesogens has also been the subject of many studies because dimers exhibit different mesomorphic behaviour then their monomeric units. Dimers of bent-core materials frequently showed significant dependence of mesomorphic properties on the type and length of spacer connecting the monomeric units through the terminal flexible chain (end to end).

In this preliminary contribution, we present synthesis and mesomorphic behaviour of innovative series of bent-core dimers in which the monomeric bent units are connected head to head (Figure 1). To prevent the general structure of bent-core materials based on resorcinol and to connect both monomers together by an alkylene unit, benzene-1,2,3-triol and benzene-1,3,5-triol as central cores were utilized. The mesomorphic properties of the new dimers were tuned by various combinations of cores, length of the spacers (n), and type of terminal flexible chains (**R**).

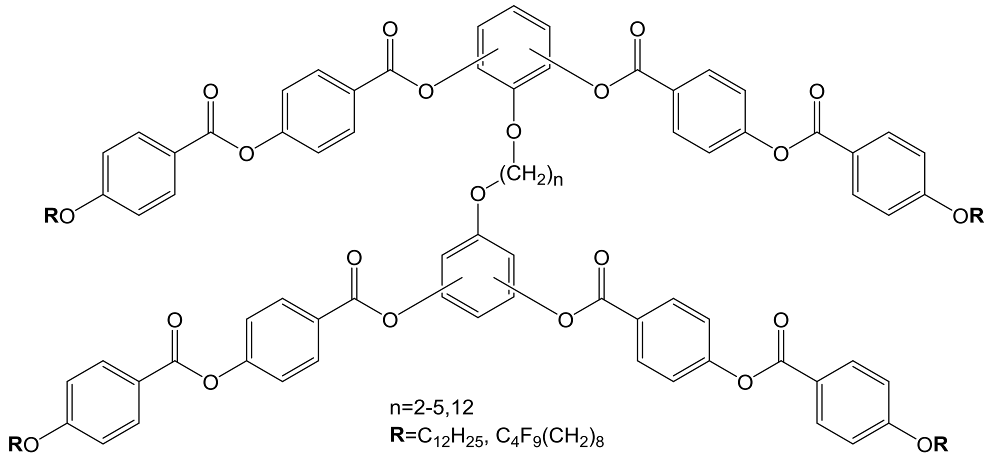

Figure 1. General structure of novel studied dimers.

Mesomorphic properties of synthesised molecules were investigated by polarising optical microscopy and differential scanning calorimetry. Their X-ray characterization is under way.

This work was supported by the Czech Science Foundation (projects No. 15-02843S, 16-12150S).

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Formation of new complex LC phases by T-shaped bolapolyphiles cores

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T-shaped and X-shaped bolapolyphiles are able to form a wide variety of new LC phases, among them various liquid crystalline honeycomb structures – with polygonal cells of different shapes ranging from triangular to hexagonal and beyond *[1]*.

Herein we report a new series of T-shaped polyphilic molecules with the structure shown in Figure 1. These compounds were synthesised and their mesomorphic behaviour was fully characterised by XRD, DSC and polarising microscopy. Depending on the side chain structure, namely the total chain volume with respect to the effective chain length, a series of very different and highly complex new LC phases was observed. The modification of the ratio between total chain volume and effective chain length was tailored for these compounds by distinct modes of branching of the lateral chains. Besides columnar phases, either with rectangular symmetry or with giant hexagonal lattice, two different types of cubic phases, and also correlated lamellar phases were found. The rectangular columnar phase forms honeycombs composed of octagonal and pentagonal cylinders in a ratio 1:2, leading to a tiling pattern resembling that of zeolites with the framework structure BIK. Moreover, this structure containing giant octagonal channels requires that these channels are filled by additional molecules. This leads to a unique LC structure which combines rod-like molecules assuming orthogonal orientations to each other *[2]*. With further increasing chain lengths two cubic phases, one with *Ia*3;¯*d* lattice (bicontinuous, double gyroid) and the other with *Fd*3;¯*m* lattice (single diamond) were found. The lamellar phases occurring besides these cubic phases represent lamellar phases with the rod-like unit arranged parallel to the layer planes; correlation between adjacent layers leads to the observed *p*2*mm* symmetry.

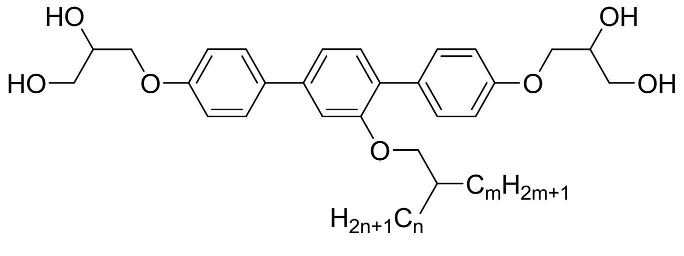

Figure 1. Structure of discussed bolapolyphiles.

The work was supported by the DFG in the framework of FOR 1145.

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An isothermal twist-bend nematic to nematic phase transition

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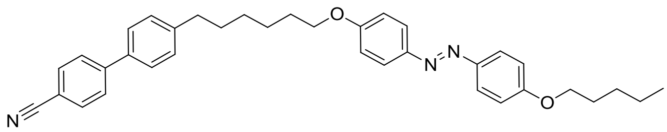
The twist-bend nematic phase (N_{tb}), has recently attracted much attention. In the N_{tb} phase the director forms a helix and is tilted with respect to the helical axis. The N_{tb} phase had previously been predicted to exist for bent molecules by Dozov and its formation attributed to a bend elastic constant (K_{33}) which tends towards zero *[1]*. It was first identified in the dimer CB7CB *[2]*.

A variety of differing molecular structures have been shown to exhibit the twist-bend nematic phase *[2-4]*. What is clear thus far is that a sufficient molecular curvature is needed in order to provide a low enough K_{33} to stabilise the phase.

Here we report the first example of an achiral dimer containing an azobenzene moiety linked to a cyanobiphenyl unit by a methylene-ether flexible spacer:



The dimer exhibits two mesophases; the higher temperature phase has been assigned as a conventional nematic phase whilst the lower temperature mesophase has been shown to be a twist-bend nematic phase. The N_{tb}-N and N-I transition temperatures are reduced upon irradiation by UV light, with the reduction in $T_{Ntb\text{-}N}$ being larger. Thus, an isothermal reversible N_{tb}-N transition may be driven photochemically. This is attributed to the *trans-cis* isomerisation of the azo linkage and provides further evidence of the critical dependence on shape of the N_{tb} phase.

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Shape minimization problems for liquid crystals

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We consider a class of problem where the configuration of a nematic liquid crystal must be found by minimizing the energy functional with respect to both internal fields as well as the shape of the domain, incorporating both local and global constraints. We present an adaptive finite-element scheme to solve these problems and explore the effect of the physical parameters on the shape. Results for other types of liquid crystal, such as cholesterics and twist-bend materials will also be discussed.

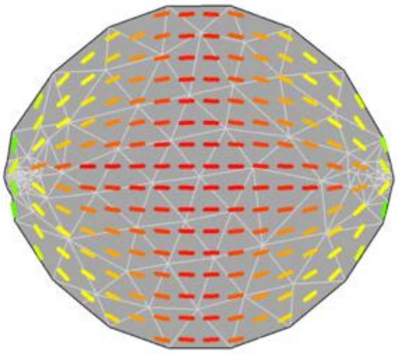

Figure 1. Sample solution for a nematic liquid crystal confined to a flexible cylinder.

Towards supramolecular complexes showing the twist-bend nematic phase

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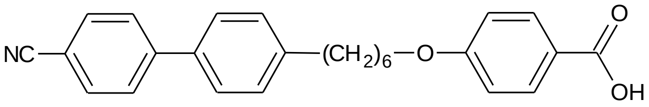
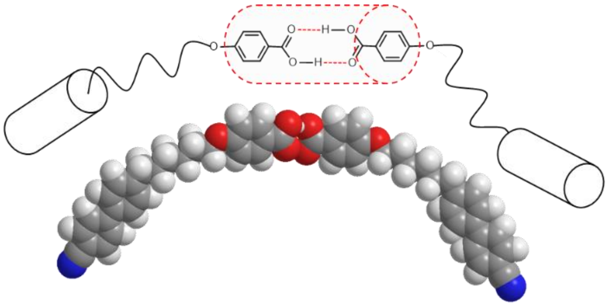
Hydrogen-bonded liquid crystals, HBLCs, continue to be the focus of much research interest as a flexible approach to obtain new functionalised mesomorphic materials *[1,2]*. Among the wide variety of different structures, H-bonding has been applied to obtain supramolecular liquid crystal dimers containing flexible spacers between either covalent or supramolecular mesogenic units *[3]*. Recently, we have reported the first case of twist-bend nematic phase, N_{TB}, stabilised by hydrogen bonding, shown by the 4-[6-(4'-cyanobiphenyl-4-yl)hexyloxy]benzoic acid, CB6OBA *[4]*.



The phase behaviour is accounted by the formation of a supramolecular trimer whose geometry is compatible with the N_{TB} phase *[5,6]*.



Attempts to extend this strategy to obtain asymmetric supramolecular complexes exhibiting the twist-bend nematic phase, however, have revealed the importance that even small variations in the structure may have on the phase behaviour of the resulting complexes *[7]*.

In the present work we review these findings by studying in detail the role of hydrogen-bonding stability on the phase behaviour of these and similar complexes. This is carried out using temperature dependent Fourier transform infrared spectroscopy, FTIR. The potential of the "soft" non-covalent bond to assist the adoption of non-linear conformers through the formation of the so-called "open dimers" is discussed.

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The effects of the mesomeric nature of the terminal group on N_{TB} phase behaviour in liquid crystal dimers

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Since the recent identification of the twist bend nematic phase (NTB) in methylene-linked cyanobiphenyl based liquid crystal dimers *[1,2],* and the confirmation of the structure using freeze fracture transmission electron microscopy *[3,4]*, interest in the NTB phase has escalated. The NTB phase was previously predicted by Dozov, who suggested that in a nematic phase the director may bend around bent dimers leading to two new nematics with nonuniform director distributions (splay-bend or twist-bend), whereby the achiral molecules are expected to form a helix in which the molecular director is tilted with respect to the helical axis in the NTB phase *[5]*.

As the NTB phase has been reported for a limited number of compounds, the development and understanding of the relationships between the molecular structure and the formation of the NTB phase are in their early stages. Previous studies have focussed on the molecular shape and the impact this has on the phase behaviour, and it is clear that molecular curvature is of fundamental importance. However, little is currently known about the effect of the mesomeric nature of the terminal groups on NTB phase behaviour.

Here we report the liquid crystalline behaviour of four dimers based on the structure shown in Figure 1. These compounds show the NTB phase. Using density functional theory (DFT), the effects that a change in the terminal unit from an electron withdrawing to electron donating group has on the electron distribution of the molecules can be visualised. We attempt to interpret the phase behaviour observed in terms of these DFT calculations.

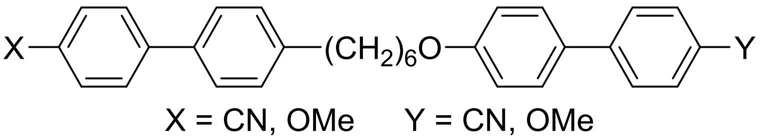

Figure 1: Molecular structure of the four liquid crystal dimers studied.

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The role of hydrogen bonding in stabilising the twist-bend nematic phase: an infrared study

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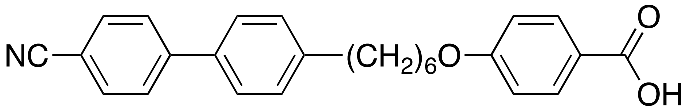
The recent discovery of the twist-bend nematic phase, N_{tb}, has caused considerable excitement. The N_{tb} was predicted by Dozov *[1]* who proposed that certain molecules may have a tendency to pack into bent structures. In the N_{tb} phase, the director exhibits periodic twist and bend deformations forming a conical helix with doubly generate domains having opposite handedness. The director is tilted with respect to the helical axis.

The N_{tb} phase was first discovered experimentally for 1′′,7′′-bis(4-cyanobiphenyl-4′-yl)heptane, CB7CB *[2]*. The study of the N_{tb} phase is still in its early stages, but it is clear that the geometry of the molecule plays a central role and in particular, the N_{tb} phase is critically dependent on molecular curvature *[3]*.

In searching for new twist-bend nematogens, we have recently reported the first example of a compound in which the twist-bend nematic phase is stabilised by hydrogen bonding, namely 4-[6-(4′-cyanobiphenyl-4-yl)hexyloxy]benzoic acid, CB6OBA *[4]*,



The phase behaviour shown by CB6OBA is accounted for by the formation of a supramolecular trimer, in which the central mesogenic unit is formed by hydrogen bonding between two benzoic acid units. It is well-known, however, that in mesophases shown by benzoic acid derivatives we see the coexistence of cyclic and open dimers, as well as monomeric (free) acids, in a complex equilibrium *[5,6]*. In the present work, we analyse in detail how the stability of hydrogen bonding in CB6OBA relates to its phase behaviour, and have performed a temperature dependent Fourier transform infrared spectroscopy study, FT-IR, with the aim of identifying the different species present, and their role in the formation of the N_{tb} phase.

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Phase behaviour of hydrogen-bonded methylene-ether linked liquid crystal dimers

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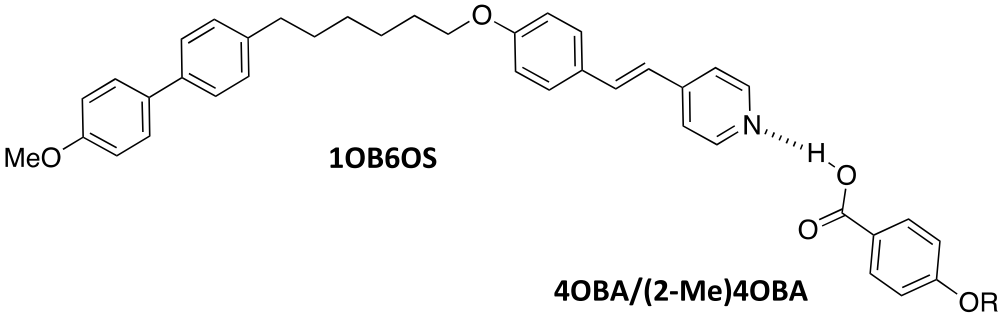
The recently discovered twist-bend nematic phase, N_{TB}, has generated significant interest since its prediction in 2001 [1]. Dozov proposed that certain molecules with a tendency to pack into bent structures can compensate for this spontaneous bend by introducing other deformations of the local director – twist or splay – and hence have the ability to form new nematic phases: twist- or splay-bend respectively. In the N_{TB} phase, the director exhibits periodic twist and maps out a helix with doubly degenerate domains having opposite handedness – giving local spontaneous chirality but an overall achiral phase. Experimentally, the N_{TB} phase has been seen in bent methylene-linked dimers, most notably CB7CB [2], as well as dimers with methylene-ether, ether, and imine linkages. It has also been observed in chiral materials [3]. The role of hydrogen bonding in stabilising the twist-bend nematic phase has been a subject of recent studies [4].

In the present work, we report the phase behaviour of bent-shaped liquid crystal dimers formed via hydrogen-bonding between unlike H-bond acceptors and donors, namely a stilbazole-based bent molecule (1OB6OS) and butoxybenzoic acid (4OBA) and chiral 2-methylbutoxybenzoic acid ((2-Me)4OBA).



1OB6OS

4OBA/(2-Me)4OBA

The complex between 1OB6OS and 4OBA exhibits a twist-bend nematic phase. Ternary mixtures of 1OB6OS and 4OBA/(2-Me)4OBA in varying proportions were used to construct a phase diagram to establish the effect of concentration of the chiral component on the formation of the N_{TB} phase.

References

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Novel resists for nanofabrication on insulating substrates

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Electron beam lithography is widely used in high value low volume manufacturing, and in research, of nanoscale electronics and micromechanical systems and nanotechnology. However, it is not possible to directly pattern poorly conductive or insulating substrates with feature sizes smaller than about 100 nm due to charging by the electrons. A number of existing strategies such as the use of charge dissipation layers or patterning of intermediate moulds have been investigated but typically add complexity and cost without necessarily significantly improving the situation. In this project, we investigate and develop photoresists using Triphenylene organic conductors to incorporate the charge dissipation strategy directly into the lithographic imaging layer. We characterise the conductivity, lithographic, etching and other properties of the new resists and investigate their performance for nanoscale patterning of substrates such as glass and gallium nitride.

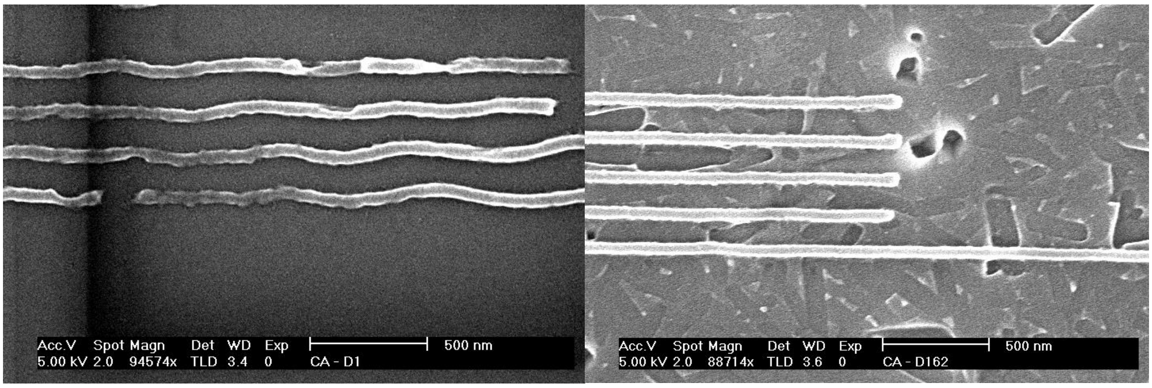

Figure 1. These images are taken after sputtering ~4 nm Gold on top of the pattern after development.
On the left at 50 µC/cm^2 a feature size of 55 nm on a 150 nm pitch are shown.
On the right at 20 µC/cm^2 76 nm features on a pitch of 200 nm are shown

Developing hole transport layers using doped triphenylene discotic liquid crystals

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Discotic liquid crystals (DLCs) form columnar mesophases [1,2]. Individual molecules typically consist of rigid poly-aromatic cores substituted with flexible alkyl chains and phase separation between the two leads to columnar packing. The electron rich cores exhibit pi-stacking hence supporting charge conduction and the alkyl chains are insulating, leading to the formation of 'molecular wires' with anisotropic charge conduction in bulk aligned mesophases [3]. DLC mesophases have been shown to exhibit high charge carrier mobility (along the columnar director), in addition to the ability to form highly ordered mesophases with either homeotropic (columnar axis perpendicular) or planar (columnar axis parallel) alignment with respect to a substrate.

Progress towards the development of hole transport layers using p-type doped discotic liquid crystals for out-of-plane conduction in devices is presented. Hexakis(hexyloxy)triphenylene molecule HAT6 is utilized as a test case[4], and both alignment and conductivity of crystalline films is studied. Binary mixtures of HAT6 and a longer alkyl-chain derivative HAT10 are utilized to study their effect on phase transition temperatures and bulk alignment of the mesophases, in particular the alignment in crystalline films prepared using spin-coated (air-interface) and capillary filled (sandwich cells) is studied. Differential Scanning Calorimetry and Polarizing Optical Microscopy are utilized to study phase transition temperatures and optical textures. In addition, X-ray diffraction and grazing incidence wide angle X-ray scattering (GIWAXS) measurements are performed and it is identified that binary mixture formation strongly affects the columnar alignment in solution processed films.

P-type doping is performed by adding varying amounts of the strong electron acceptor 2,3,5,6-tetrafluoro-7,7,8,8-tetracyanoquinodimethane (F4TCNQ) to HAT6, HAT10 and a binary mixture. It is shown that bulk conductivity of the DLC films increases by more than two orders of magnitude with dopant percentages as low as 0.1 wt.%. Both in-plane and out-of-plane conductivity is studied, and UV-visible spectroscopy, photo-luminescence spectroscopy (PL) and I-V measurements are utilized to further characterize and establish the improvement of hole conduction in the doped films. Finally, the results are discussed in relation to future applications as hole transport layers in photo-voltaic devices.

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Studying the phase behaviour of lyotropic liquid crystals using dissipative particle dynamics

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Dissipative particle dynamics (DPD) simulation has developed as a powerful predictive tool over the past two decades, allowing one to readily simulate at the mesoscale with simplified coarse grained models. The focus of this study is to parameterise the DPD coarse-grained unit in a chemically tractable manner to reproduce the phase behaviour of lyotropic liquid crystals.

Groot and Warren *[1]* outlined a simple approach to map DPD to specific chemical identities via Flory-Huggins theory, which remains widely used in current practice. However, in our implementation of this parameterisation we find flaws that make it unsuitable in producing representative models of surfactants.

Through the use of solubility data *[2,3]*, we have successfully developed models of typical anionic surfactants that reproduce phase progressions with respect to concentration. As an example, figure 1 illustrates our coarse-grained model of an isomer of linear alkylsulphate (LAS) and its reproduction of the lamellar phase at high concentrations.

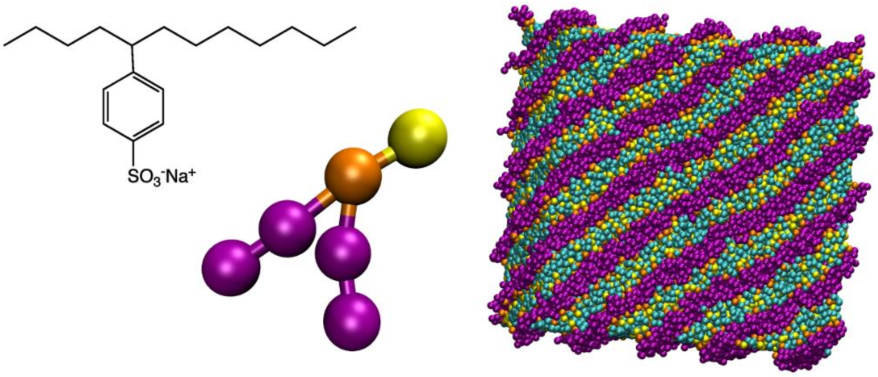

Figure 1: left is the structure of LAS, centre is our model, and right is the lamellar phase produced at 80% volume LAS.

Building on our successful parameterisation for anionic surfactants in water, we intend to reproduce the phase behaviour of mixtures of lyotropic liquid crystals in a series of solvent models; and to investigate which interactions of typical additive molecules (e.g. perfumes, chelants) give rise to changes in the phase behaviour and stability of the lyotropic mesophases.

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Multiscale computer simulations of an anionic chromonic dye

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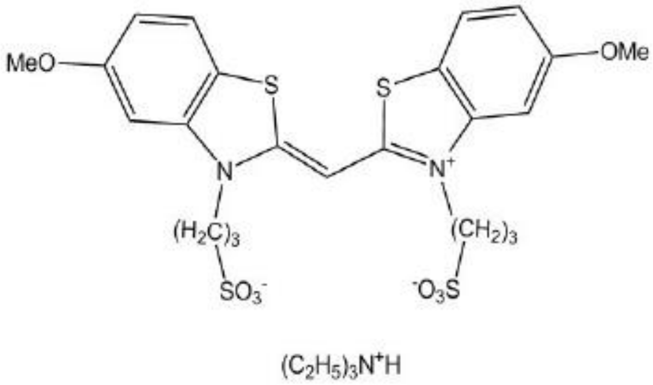
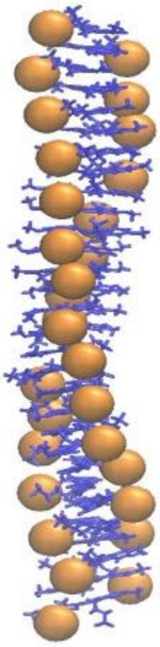
Controlling self-assembly of nanostructured soft matter in aqueous solution is of considerable interest in the formation of thin organic films and in future organic electronics applications.

A rare "self-assembled" motif, named the double-width column structure has been proposed to interpret experimental findings for the anionic chromonic dye (shown left). Higher concentrations are proposed to form a novel biaxial smectic structure. However, the vast majority of chromonic mesogens favour a direct face-to-face aromatic stacking arrangement, causing some controversy as to whether either of these proposed models is energetically feasible.





The formation of a chromonic liquid crystal phase deals with phenomena covering a wide range of length and time-scales, from the short-range interactions between chromonic mesogens to form an aggregate, to the long-range movement and alignment of columns to form a phase. A range of different computational methods need to be implemented to probe the different level of description required for a system.

Molecular dynamics simulations can provide a molecular level picture of the preferred stacking structure within chromonic aggregates in aqueous solution. Here, direct simulation of atomistic models in water, in which all interactions are accounted for (including long range electrostatic interactions), allow for direct observation of selfassembled aggregates and phases.

Coarse grained models, where the degrees of freedom are reduced by incorporating several atoms into a single bead with a new potential, allow for direct observation of larger scale self-assembled aggregates and phases.

Atomistic simulation results will be presented showing the formation of chiral aggregates at low concentrations (see figure right) and a novel layer structure on increased concentration, together with an attempt to systematically generate a coarse-grained model system.

This work is supported by the UK research council EPSRC and Durham University through a DTA studentship award.

Synthesis of staggered triphenylene twins linked through ferrocene bridges

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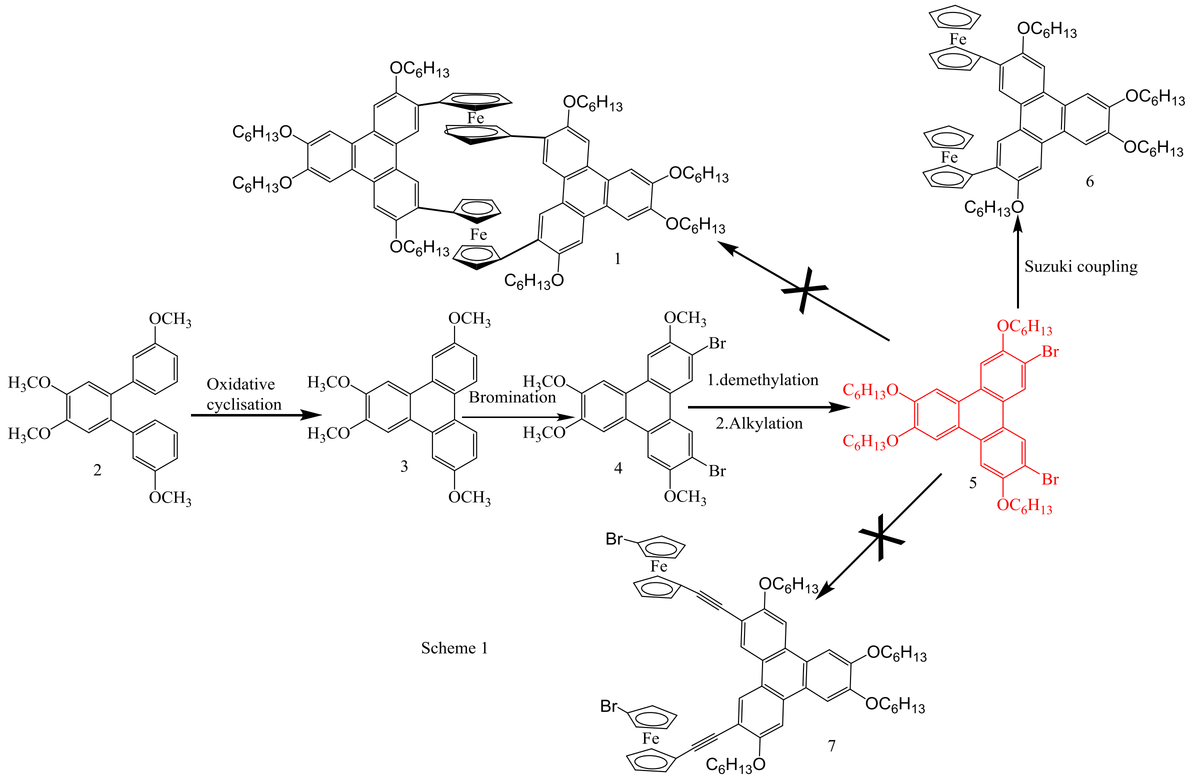
Interest in the chemistry of triphenylenes has increased rapidly over recent decades. The triphenylene core is one of the most important systems for discotic liquid crystals (discogens) *[2]*. Many different strategies are now known for the synthesis of substituted triphenylenes, allowing control over the number and position of different side groups *[1]*. Further synthetic progress has developed pathways to different symmetrical and unsymmetrically substituted derivatives *[3]*. Twinned systems have been shown to display unusual mesophase behaviour.

This project aims to investigate a new architecture in twinned systems whereby the link imposes a stagger between the discogens. Our research work focuses on the synthesis of new twinned triphenylenes (alkoxytriphenylenes), **1**. A new synthesis of the precursor triphenylene **5** is presented along with model studies on the twinning reactions between triphenylene and ferrocene.



Scheme 1

References

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Synthesis and characterisation of new twinned triphenylenes

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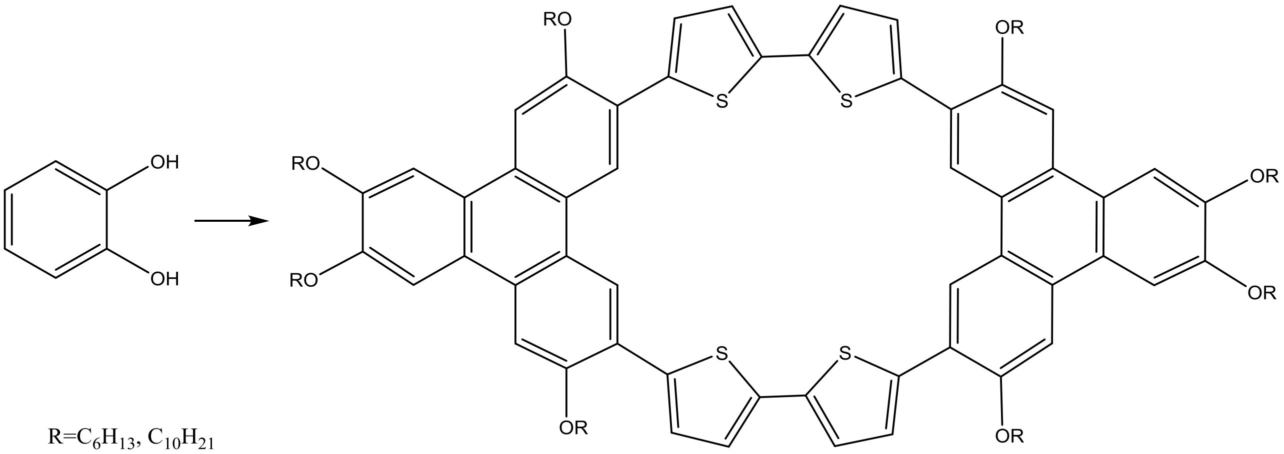
Discotic (disc-like) molecules have applications in different fields such as organic electronic devices. Their molecular structures typically have a rigid aromatic core and flexible peripheral chains *[1]*. Triphenylenes, one of main classes of discotic cores, have been most widely used in discotic liquid crystals *[2,3]*. Our group has recently embarked on a programme to investigate the effect of twinned disc-like structures through antiaromatic and aromatic conjugation pathways *[4,5]*. Antiaromatic dehydroannulene twins self-assemble to form fluid nematic liquid crystal phases *[4]*. In this project, we synthesised further twinned structures to unravel the structural features governing liquid crystal properties.

In this poster we present the synthesis and preliminary characterisation of twinned-triphenylenes. The target structure is shown below, where the two units are twinned directly *via* bis-thiophene bridges. These thiophene-based materials appear to be highly fluorescent and are therefore potentially useful in optoelectronic devices *[6]*.



Scheme 1

References

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High repetition rate liquid crystal lasers

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The maximum pulse repetition rate and average power of dye-doped chiral nematic liquid crystal (LC) lasers are limited, due to effects such as dye-bleaching and director reorientation *[1]* that reduce the laser efficiency. These performance limitations mean that LC lasers devices are currently unsuitable for many applications. This study demonstrated a method of enabling LC lasers to be operated higher repetition rates and average powers by spinning the LC laser cell at a high frequency, with the aim of creating a more versatile laser system with improved performance.

A prototype spinning system was evaluated with a band-edge LC laser. An improvement in the maximum average power was demonstrated through monitoring the energy of the laser pulses. It was found that pump frequencies greater than 3 kHz could be used with only a slight reduction in the laser efficiency; this represents an order of magnitude increase over a static cell. As expected, spinning the cell increased the stability of the emission power *[2]*, but also resulted in a small variation in the wavelength of the laser line due to the excitation of different chiral domains.

A summary of the key performance parameters of the spinning LC laser system will be presented and its limitations discussed. Possible application areas for such a system include microscopy and high throughput sensing.

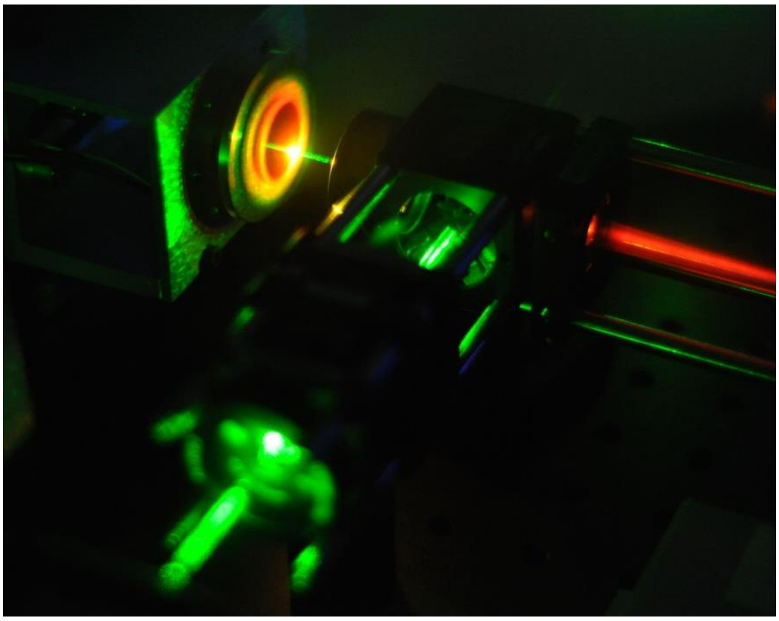

Figure 1. The spinning liquid crystal laser system in use with a green pump laser. The emission from the LC laser can be seen in red (right of image).

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Synthesis and properties of asymmetric dimeric materials with lateral and terminal fluorine substituents for DFLC mixtures lasers group

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With the continuing requirement for faster switching times an alternative route has been found in dual frequency liquid crystal materials (DFLCs). Usually DFLC materials are a two component mixture, positive compounds with a positive dielectric anisotropy that decreases at higher frequencies and negative compounds with a large negative dielectric anisotropy that remains almost constant across different frequencies *[1]*. The aim of this research is to investigate whether these two components can be combined into a single dimer material that is viable for DFLC. A liquid crystal dimer is a material with two mesogenic core units separated by a flexible spacer, usually alkyl chains. Dimers have been the target of a great deal of research due to the unusual liquid crystal behaviour they exhibit *[2]*.

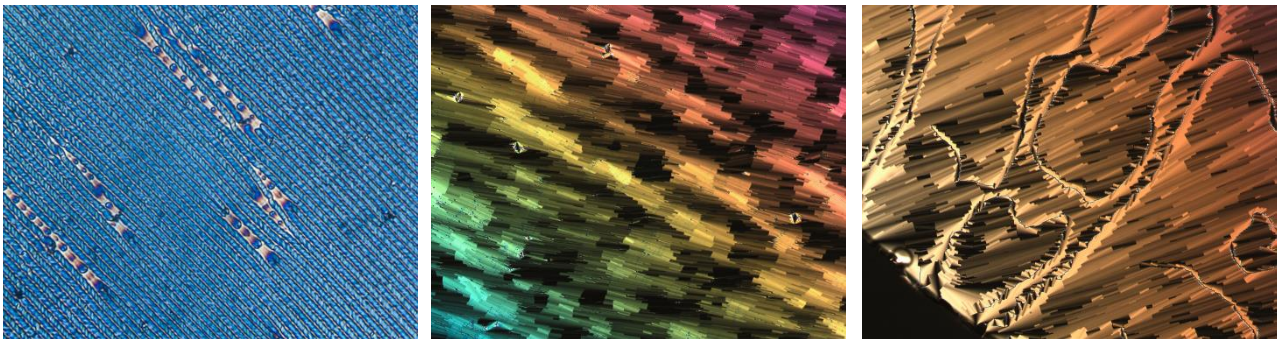
(a) (b) (c)

Figure 1. (a) rope texture of the N_X phase for a bent dimer, (b) & (c) textures seen for the linear analogue.

A series of asymmetric dimeric materials have been targeted, these feature one core unit with lateral fluorine substituents and the other core with terminal fluorination. Both odd and even spacer lengths, and the length of the mesogen cores are investigated. The mesomorphic properties have been characterised by OPM, DSC and XRD. Additionally electro-optic properties, including birefringence & frequency response have been investigated for two compounds. The vast majority have broad intercalated smectic phases with some nematic character. One material exhibits a nematic-nematic transition and possesses the N_X/N_{TB} phase. (Figure 1(a)). The linear analogue displays some unusual OPM textures (b) & (c).

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Investigation of the liquid crystal and photochromic properties of a functionalised HABI dimer group

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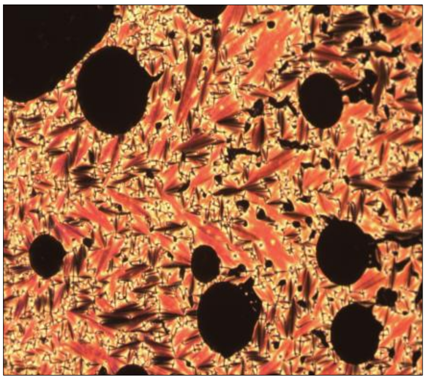
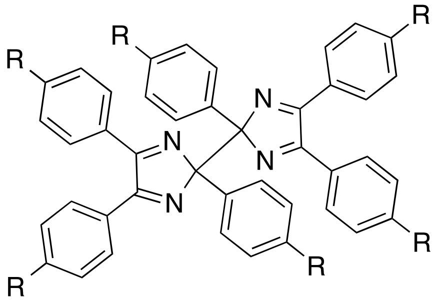
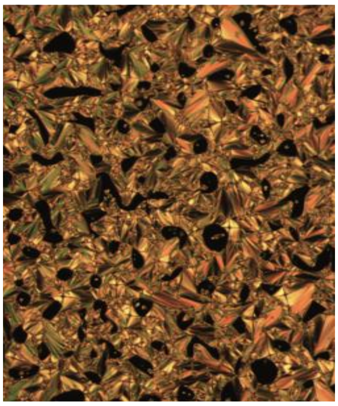
In recent years a range of photochromic molecules have been used to modulate the liquid crystal as well as the absorption behaviour of mesomorphic systems in response to light. The most often used photochromic reaction with light is the cis-trans isomerisation of bonds, such as in azobenzenes. Other reactions include the cyclisation of diarylethenes or the opening of heterocyclic rings in naphthopyrans. The simple cleaving of bonds by irradiation or pressure in the 2,4,5-triphenyl imidazole dimer used as a photochromic core functionalised with liquid crystal moieties has yet to be explored fully. The reversible change in the structure and shape of photochromic molecules has promising applications in data storage and optical devices.

In this contribution we report on our efforts on the design, synthesis and investigation of photochromic liquid crystals based on 2,4,5-triphenyl imidazole dimers *[1,2]*. The molecular construction is based on a spacer concept where the liquid crystal mesogen is attached to the photochromic core by a flexible hydrocarbon spacer. The effects of changing the spacer length, the linking group connecting the hydrocarbon chain to the imidazole core and the liquid crystal moiety, for which a cyanobipenyl group was selected, were explored in order to control the photochromic properties and the liquid crystal phase behaviour. The structure of the photochromic group will be discussed based on the 13C NMR data [3] and supported by the XRD data for the liquid crystal phase. The synthesis of a range of materials will be presented and the results of the investigation of the liquid crystal properties based on OPM, DSC and XRD experiments will be shown and the structure properties relationships will be discussed.





R = link to LC group



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Tuning the colour and phase stability of chiral nematic polymers and elastomers

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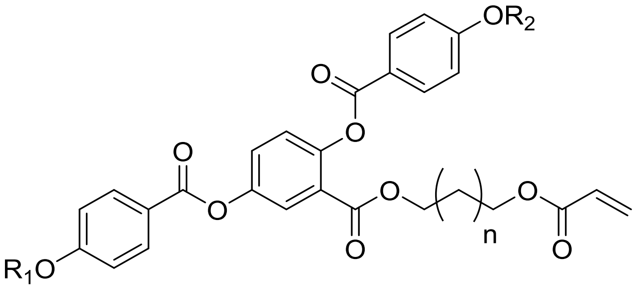
The ability to permanently capture the helical macrostructure, and therefore the unique optical properties of the N* phase, makes chiral nematic polymers of great interest. Extending this to elastomers, by light crosslinking, allows materials capable of reversible tuneable colour to be realised *[1,2].*



R_1 = $-C_4H_9$
$-C_7H_{15}$
$-CH_2C^*H(CH_3)C_2H_5$
R_2 = $-C_4H_9$
$-C_7H_{15}$
$-CH_2C^*H(CH_3)C_2H_5$
n = 2, 9

Figure 1. The structure of the chiral laterally attached side chain acrylate monomers

We have prepared a series of chiral nematic acrylate monomers as shown in Figure 1. Acrylates are an attractive choice for exploring liquid crystal polymers and elastomers due to their relatively flexible backbone, leading to low glass transition temperatures and, consequently, good nematic phase range. Achiral monomers of a similar architecture, with laterally attached mesogens, have previously been prepared and are well understood *[3, 4].* Inserting a chiral centre into the terminal alkyl chains induces an N* phase which is influenced by the position of the chiral centre, while changing the methylene spacer length further affects the glass transition temperatures of the polymers.

Photo-polymerisation of aligned monomer films with the photoinitiator Irgacure TPO and exposure to UV light produced polymer films. Their thermal and optical properties were characterised by DSC and optical microscopy. To tune the selective reflection into the visible spectrum mixtures of the chiral and achiral nematic monomers were prepared and then co-polymerised. Lastly an elastomer film containing 10% crosslinker was made and investigated.

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Double-layered liquid crystal devices with an intermediate layer

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Stacking two independently aligned liquid crystal layers has the potential for polariser free operation devices. For example, highly reflective guest-host displays use a double-layered design, in which independent layers are stacked with alignment in either layer orientated perpendicular to one another and incident light is fully extinguished using a high order parameter pleochroic dye. Such devices require the separating structure in the device centre to be as thin as possible to reduce the effect of parallax on the off-axis viewing. M. Hasegawa et. al. improved upon this design by separating two liquid crystal layers within a single cell by suspending mylar film on top of photo-resist spacers *[1,2]*. However, the separating layer increases the switching voltage and thickness of the device through the relationship:

$$\frac{V_{LC}}{V_D} = \frac{\varepsilon_S d}{(\varepsilon_D d + \varepsilon_{LC} t)}$$

where d is the cell gap, t the thickness of the separating layer, and ε_{LC} and ε_S are the permittivities of the liquid crystal and separating layer. This shows that, despite reducing the mylar thickness to 1.3µm, over 50% of the voltage for such devices is lost.

A similar design is considered for recently investigated liquid crystal contact lenses *[3-5]*. Such contact lenses also require two cavities with orthogonal alignment to obtain polarisation independent operation. In addition to the voltage requirement, it is also essential that the overall device thickness is kept well below 300µm for wearer comfort. Various devices are demonstrated for an optimised double-layered liquid crystal device where the thickness of the separating layer is reduced considerably to achieve negligible voltage loss. Also, the effect of different materials for the separating layer is considered to optimise the device design. It will be shown that this mode has major applications for improved display devices and new modes, such as liquid crystal contact lenses.

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Opening the possibilities of room temperature applications of poly(acrylate) liquid crystal elastomers

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Liquid crystal elastomers (LCEs) have vast potential in bioengineering and physical applications due to their unique coupling of anisotropy and the liquid crystal (LC) director to a cross linked elastomer matrix. Attractive properties include >300% length changes in response to stimuli, stress controlled LC director orientation and so-called 'soft elasticity' *[1-3]*. Most commonly LCEs are synthesised from, either poly(siloxane) systems via the Finkelmann 2-step method, or from poly(acrylate) systems using radical photo-polymerisation *[2,4]*.

Poly(siloxane) systems typically have a low glass transition temperature (T_g) and hence are suitable for many room temperature applications *[2]*. However, their synthesis route limits director configurations to align with an applied stress. Conversely poly(acrylate) LCEs may have complex director geometries controlled via surface or field effects *[4]*. For example it has been shown that magnetic fields and photo-alignment may be used in creating synthetic variable irises and novel actuators respectively *[5,6]*. However, poly(acrylate) LCEs typically have higher glass transition temperatures than poly(siloxane) LCEs making them unsuitable for room and body temperature applications *[7]*.

This study has investigated the addition of functional components to poly(acrylate) in an effort to reduce the glass transition temperature while still maintaining the attractive properties of poly(acrylate) LCEs. The success of this work opens the application of poly(acrylate) LCEs to room temperature environments and further removes the need for heated environments when developing and testing LCE based devices.

Outcomes

- Successfully able to control T_g to below room temperature, confirmed via DSC,
- Director alignment of low T_g LCEs demonstrated,
- Observed stress induced alignment of polydomain LCEs and director rotation in monodomain samples,
- Impacts of comonomers on mechanical properties qualitatively explored.

This research is supported through a CASE award from the EPSRC and UltraVision CLPL and through an Industrial Fellowship from the Royal Commission for the Exhibition of 1851.

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Polymers under geometrical confinement

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Spatial organisation is one of the most important features in confined spaces, like organisation of chromosomes inside the nucleus where heterochromatin and euchromatin are organised at periphery and in the middle of nucleus respectively. Using molecular dynamics simulation, we investigate the effect of confinement on a system that comprises several stiff segmented polymer chains where each chain has similar segments, but length and stiffness of the segments vary among the chains which makes the system inhomogeneous. The translational and orientational entropy loss due to the confinement plays a crucial role in organising the chains which can be considered as an entropy-driven segregation mechanism to differentiate the components of the system, like an *entropic chromatography*. Due to the inhomogeneity, both weak and strong confinement regimes show the competition in the system and we see the segregation of chains as the confining volume is decreased, Fig. 1. In the case of strong spherical confinement, a chain at the periphery shows higher angular mobility than other chains, despite being more radially constrained. The results are in qualitative agreement with the chromosome organization inside the nucleus *[1]*.

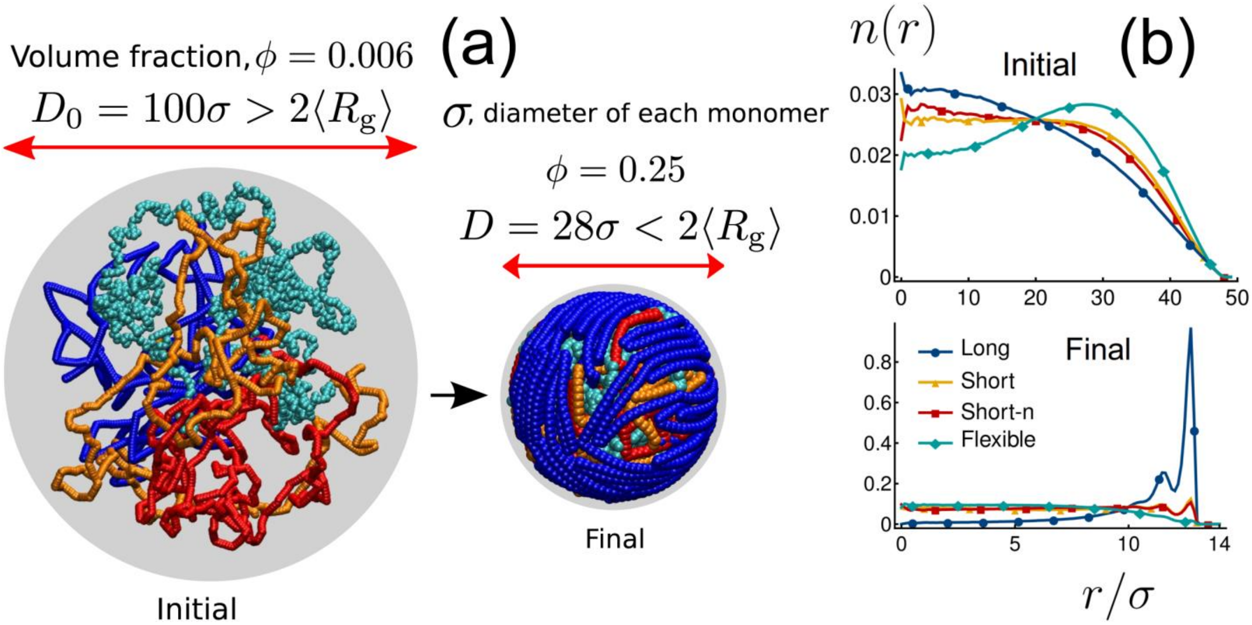

Figure 1: (a) Schematic representation of the segmented chains and the confining geometry. (b) Number density distributions. Both (a) and (b) represent the segregation of chains in strong confinement regime based on the length and stiffness of the segments

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Solvent effects on chiral nematic self-assembly of cellulose nanocrystals

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Currently photonic films prepared by drying chiral nematic suspensions of cellulose nanocrystals (CNCs) attract strong scientific interest, as these are low-cost, sustainable and highly functional materials *[1,2]*. However, the understanding of the basic physical chemistry that governs the behaviour of CNC suspensions is still highly unsatisfactory. Up to now many different approaches for altering the properties of the CNC suspensions have been investigated, often rather unsystematically, e.g. addition of salts, variation of preparation processes or chemical modification of the CNC surface. One important factor that has hardly been studied is the nature of the liquid used as host. There are only few reports on the possibility of suspending pristine CNCs in non-aqueous solvents *[3,4]* and none addresses the effect on the liquid crystal formation. The main reason for this serious knowledge gap is most likely the challenge in re-suspending the CNCs in a non-aqueous solvent.

To fill this gap we developed a new method for exchanging the solvent without modifying the CNCs or causing their agglomeration, studying the dispersion in systematically chosen polar solvents: water, formamide and *N*-methylformamide. Thus, we are able to report for the first time how the solvent influences the liquid crystal-forming properties of CNCs. As source, treatment and length distribution of the CNCs are the same for every suspension, the detected differences can readily be attributed to the difference in solvent properties. We found significant differences concerning the phase diagram, the value and concentration dependence of the chiral nematic pitch (Figure 1) as well as the time needed for the helix development. To a large extent the effects can be explained by the differences in relative permittivity of the solvents, which is thus a major influence factor on the characteristics of the CNC suspensions. With these investigations we contribute to an enhanced understanding of the fundamental physical chemistry of CNC suspensions, opening up new possibilities to tune their properties.

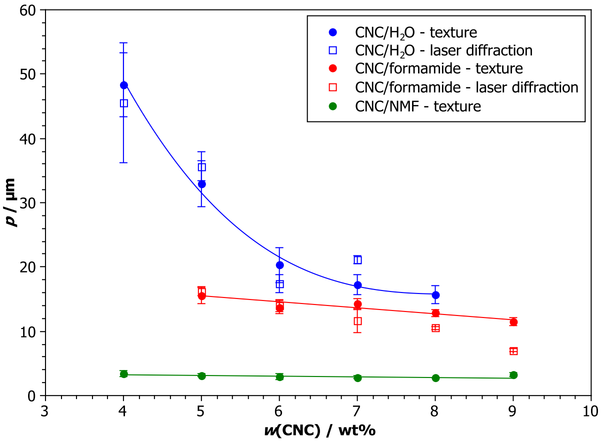

Figure 1. Chiral nematic pitch of CNC suspensions with different solvents.

Financial support by the Dr. Leni Schöninger Foundation and the Luxembourg National Research Fund (grant code C14/MS/8331546) are gratefully acknowledged.

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Photomanipulation of the anchoring energy and its effect on the behaviour of LC colloids

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Recently, photo-switchable azo-dendrimers spontaneously adsorbed at glass/LC interfaces have been shown to switch reversibly between homeotropic and planar anchoring conditions when exposed to UV [1-3]. In colloidal LC systems, this effect results in the photo-switching of the director field in the vicinity of LC droplets, or even mechanical motion of the colloidal particles in the nematic matrix [4,5]. We demonstrated that these effects are determined by a light-driven change of the anchoring energy of the glass/LC interface [4].

Here, we report measurements of the interfacial surface tension anisotropy (anchoring energy) at an ITO-glass/5CB interface under exposure to UV and VIS light illumination. We demonstrate that the anchoring strength depends on the ratio of the intensities in the UV and VIS bands. A simple model is developed to qualitatively explain the dependence of the anchoring energy on the light intensity. These results are then applied to describe the light-driven kinetics of the opto-mechanical effect which has been explored in the dependence of both UV and VIS illumination. Additionally, we report the structure and the order in the dendrimer layer at the glass/LC interface. Using Second Harmonic Generation and Attenuated Total Reflection IR Spectroscopy, it is shown that the dendrimer molecules adopt a polar structure, which can be reversibly suppressed by the UV illumination, and restored by the VIS illumination. Unusual behaviour is found in liquid crystalline droplets in an isotropic matrix. In case of bent-core nematics, the droplets with the LC/dendrimer mixture exhibit a spiral texture in polarising microscopy. We show that the spiral handedness can be switched by exposure to UV. We discuss a possible director configuration which can explain this behaviour.

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Microrheology of isometric and anisometric particles in a 2D fluid

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Fluid systems in reduced geometry are found both in nature and in artificial devices. Diffusion of protein complexes in biological membranes, as examples of 2D fluids, is related to a mobility that cannot be described by 3D hydrodynamics [1,2]. One of the exciting features of 2D fluids is the Stokes paradox: a translational mobility, describing the relation between viscous forces and terminal velocities of inclusions, cannot be defined. There is no steady state solution of the slow viscous flow equations for translational motion in 2D. A theory of 2D hydrodynamics has been developed for isometric particles by Saffman and Delbrück *[1]*, refined by Petrov and Schwille *[2]*, and recently extended for rod-shaped particles by Levine et al. *[3]*.

Here we report measurements of translational and rotational mobilities originating from viscous forces in freely suspended smectic films, which are ideal models for 2D fluids. Smectic-A films represent 2D isotropic fluids, and smectic-C films model 2D nematics *[4]*.

When the lateral film size is smaller than the Saffman length Ls, isometric particles (glass spheres) as well as anisometric particles (glass rods) exhibit a confinement-driven dynamics. In the opposite case, the motion is determined by viscous coupling to the surrounding air. We demonstrate that the motion of rods with the length $L \ll Ls$ is independent of the rod orientation and can be well described by the Petrov-Schwille approximation *[2]*. When the length of the rods is comparable to Ls, the drag force becomes anisotropic. The drag $\zeta\perp$ for motion perpendicular to the rod axis becomes larger than the drag for the parallel motion, $\zeta\|$. We discuss the dependence of the two drag coefficients $\zeta\|$ and $\zeta\perp$ on the rod length and the aspect ratio as well as behaviour of the rotational drag ζ_r in the light of the theory of Levine et al. *[3]*.

In smectic C, even isometric inclusions couple to the c director field of the films in a complex way. When such a particle moves down the film plane in an inclined smectic film, it creates a wake consisting of walls of the c director field. The film orientation in front of the moving inclusion, however, has no measurable influence on the speed in that 2D rheology experiment.

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Synthesis of micrometer-sized photoresponsive actuators based on liquid crystalline elastomers (LCEs)

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The use of liquid crystalline elastomers for actuator applications has been reported for several years. When the mesogens in a crosslinked liquid crystalline polymer change their orientation during the phase transition from the LC phase into the isotropic phase, the polymer backbone is allowed to change from a stretched into a coiled conformation, which results in an overall deformation of the material.

To realise strong shape changes, it is necessary to orient the mesogens into a liquid crystalline monodomain before the polymer is crosslinked. Using microfluidics is the best known method to fulfill this condition of oriented mesogens in particles and to synthesis those in a continuous flow with control over size and shape. Applying this method; thermoactuating particles were already synthesised in our group which showed a length change of more than 70% when they were heated above the clearing temperature *[1]*. However, a thermal actuation is not favourable for an application in devices because the whole surrounding needs to be heated up. So actuation induced in a more practical way is desired.

Here we present the fabrication of photoresponsive particles that change their shape by irradiation with UV-light. Therefore, we use an azo-group containing LC-monomer (Fig. 1c) and a LC-crosslinker which are polymerised by a VIS-photoinitiator in a microfluidic device. (Fig. 1a)
With the same monomer, but a non-LC-crosslinker Keller et al. produced photoactuating films already, which showed a photo induced change of length of up to 17% *[2]*. For the particle synthesis the monomer mixture is melted and injected through a very thin needle into a co-flowing stream of silicone oil. The resulting droplets are first cooled into the liquid crystalline phase, polymerised with red light further downstream, and then collected at the end of the tube. Appling this method, LCE particles were produced which change their length by up to 24% in seconds under irradiation with UV-light (Fig. 1b), while a back deformation taking about 8 minutes can be achieved by irradiation with red light.

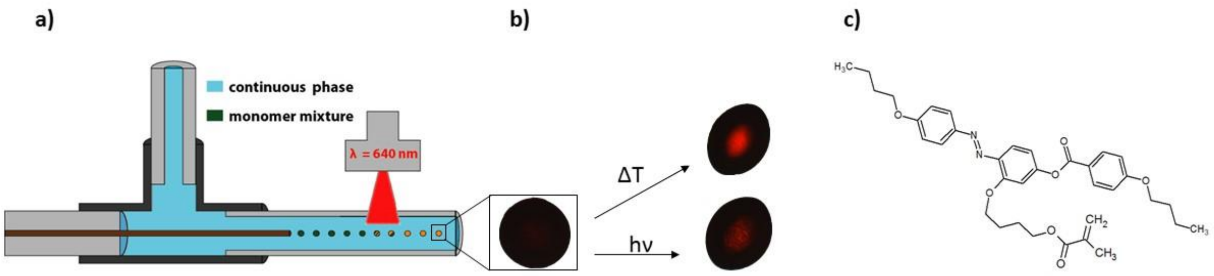

Figure 1. a) Microfluidic set-up for the particle fabrication, b) an actuating particle and c) used monomer.

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Crosslinking of liquid crystalline nanoparticles

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In this work we want to present a method to construct responsive and non-equilibrium nanomaterials that can change their internal structure through external stimuli.

For that reason we have functionalised titanium dioxide nanorods with statistical N-isopropylacrylamide and benzophenone-based crosslinker copolymers that were synthesised through reversible addition-fragmentation chain transfer polymerisation. It is possible to attach polymers to nanoparticles with a poly(pentafluorophenyl acrylate) anchor block *[1]*.

The functionalisation of the particles prevent agglomeration in suitable solvents through steric interactions. The nanoparticles, which act as mesogens, are flexible and can build lyotropic and thermotropic liquid crystalline phases *[1]*.

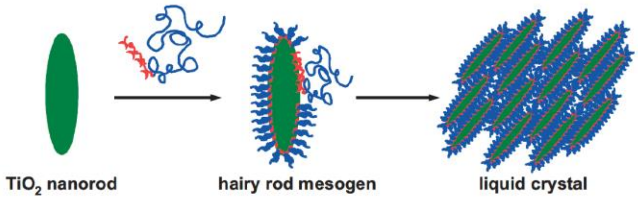

Figure 2: Functionalisation and orientation of titanium dioxide nanorods *[1].*

By crosslinking the nanoparticles with the help of benzophenone groups through irradiation with UV-light it is possible to “lock-in” a memory of the order during the network formation.
A liquid crystalline order, for example, can be destroyed through a phase transition in the isotropic state by raising temperature.

The thermoresponsive poly(N-isopropylacrylamide) shows a lower critical solution temperature of 32 °C in water *[2]*. So the network shows different grades of swellability in dependence of temperature, but also in dependence of solvent and the degree of crosslinking. Hereby these are other possibilities to disturb the state of order of the used mesogens.

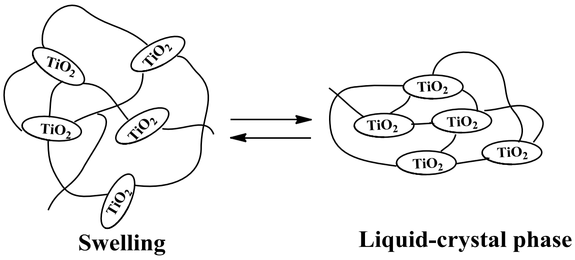

Figure 2: Swellability of a polymer network.

We could show that it is possible to build liquid crystalline phases with functionalised titanium dioxide nanorods by polarized optical microscopy. Furthermore, we have attached polymers with different chain and anchor block length to titanium dioxide nanoparticles and crosslinked them afterwards. We also could determine the degree of swellability in dependence of temperature in water and of solvent with a quartz crystal microbalance.

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Liquid crystalline phases of magnetite nanorods

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The formation of liquid crystalline phases is experimentally and theoretically well-investigated for rigid-rod objects, like form anisotropic inorganic nanorods with high aspect ratio *[1]*. Liquid crystalline phases will be formed spontaneously above a certain threshold concentration. This requires the mobility of the nanometer-scale objects at high concentration. Thus, a neat material of highly anisotropic nanometer-scale objects does not usually form LC phases owing to lack of mobility. This requires the "solubilisation" of the nanometer-scale objects. Therefore, the concept of "hairy" rods, which was originally developed for stiff main-chain LCs, is promising *[2].* In this model, a stiff insoluble core is solubilised by long alkyl chains (the hairs) on its surface. The applicability of the concept has already been demonstrated for anisotropic nanoparticles *[3].*

Form anisotropic magnetite (Fe_3O_4)-nanorods were surface functionalised with P(MMA-*b*-dopamine) block copolymer and the lyotropic liquid crystalline behaviour was investigated. The synthesis of the block copolymer consisting of a PMMA solubilisation block and a dopamine anchor block was realised by radical addition fragmentation transfer (RAFT) polymerisation via a macro-initiator approach. Functionalised magnetite nanorods could be dispersed in organic solvents. By solvent evaporation (increase of nanorod concentration) birefringent domains appeared. Under the additional influence of an external magnetic field a uniform orientation of the birefringent domains was obtained. Further investigations were done in PEG 400 as non-evaporating solvent and dispersions of the functionalised nanorods were observed. Under the influence of a magnetic field the nanorods aligned along the external field and a phase separation into a lyotropic LC phase rich in anisotropic objects and an isotropic phase lacking of anisotropic objects was obtained. After removal of the external magnetic field, the nanorods self-assembled themselves in three-dimensional "net-structures" with a director along the previous structures. By a demagnetiser the alignment was reversible, therefore only dispersed nanorods were obtained again.

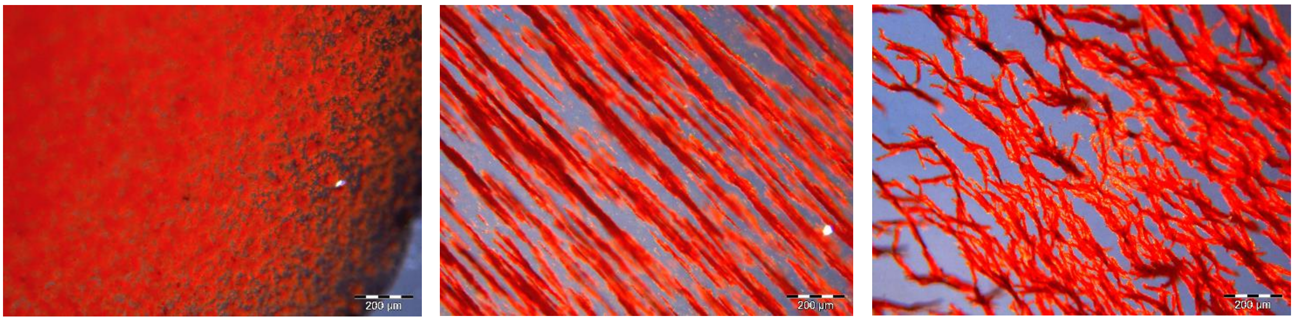

Figure 1. Functionalised nanorods dispersed in PEG 400 without external field, under the influence of an external magnetic field and after removal of the external magnetic field (from left to right).

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Synthesis of discotic liquid crystalline tristriazolotriazines and studies of their optical and thermotropic behaviour

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Generally composed of a rigid core and flexible side chains, thermotropic liquid crystals (LCs) form an important category of soft matter with a unique combination of molecular order and dynamics *[1]*. Star-like molecules with small central rings and π-conjugated arms with flexible side chains can also build discotic LC phases *[2]*. Due to one-dimensional charge-carrier transport in those assembled columnar superstructures, the materials are applicable in organic field-effect transistors and photovoltaics *[3]*.

Synthetic and structural studies of tristriazolotriazines with a threefold dialkoxyaryl substitution indicate that thermotropic properties and organisation of the systems can be well regulated by the steric demand of the aryl groups *[4]*. X-ray studies show a highly complex helical superstructure at increased temperatures. These compounds furthermore show negative or inverted solvatochromism of the UV/Vis absorption and a strongly positive solvatochromic behaviour of their fluorescence.

The method of Huisgen et al. is currently the only synthetic approach to tris-[1,2,4]triazolo[4,3-a:4,3-c:4,3-e][1,3,5]triazines (TTTs) *[5]*. Acylation of tetrazoles with cyanuric chloride followed by thermal elimination of nitrogen and ring closure results in TTTs in good yields.

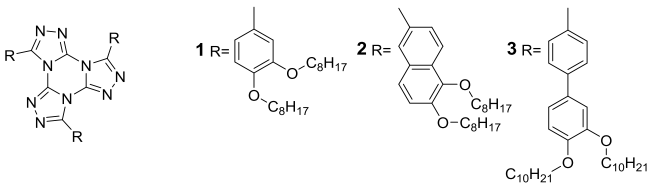

Fig. 1: Structures of the studied materials.

The thermotropic properties of the three disc-like molecules (Fig. 1) were characterised by polarized optical microscopy (POM), differential scanning calorimetry (DSC) and wide- and small-angle X-ray scattering (WAXS and SAXS). Cooling the isotropic liquid phase of TTTs 1-3 into an enantiotropic liquid-crystalline phase (10 °Cmin^{-1}), POM indicates characteristic pseudo-focal conic fan-shaped textures which indicates a discotic hexagonal columnar phase (Colh) *[6]*. Investigations of TTT 1 and TTT 2 with POM indicate dendritic growth by slow cooling (1 °Cmin^{-1}). Whereas both phase transitions, melting and clearing could be observed for TTT 1 and TTT 2 by POM and DSC, the DSC of TTT 3 shows only the clearing transition.

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Dielectric relaxation behaviour of graphene-oxide micro-flakes in isotropic and nematic solvents

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The experimental results of lyotropic nematic liquid crystals (LC) formed by graphene-oxide flakes (GO) in various solvents, and the behaviour of the dielectric relaxation of the GO in the different media and for different flake sizes were investigated. GO is a one or few-atomic-layer thick material, produced by the exfoliation of graphite oxide, decorated with hydroxyl and epoxide functional groups on the surface and carbonyl and carboxyl groups at the edges of the sheet. The self-assembly and the interface-to-interface interactions of GO sheets stimulated the formation of lyotropic nematic liquid crystalline domains in the isotropic medium, or solvents *[1]*. In an anisotropic medium, such as a thermotropic nematic phase, the GO flakes arranged under the nematic orientational order. Upon heating and transforming the nematic medium to isotropic, the GO flakes arrange and experience the medium as an isotropic solvent, thus forming a lyotropic phase.

Previously, one-dimensional particles such as carbon nanotubes have been found to affect the collective dielectric modes in ferroelectric liquid crystal *[2]*. Here the ultra-high dielectric constant of GO has encouraged us to carried out a systematic dielectric study of the GO suspensions to deduce the microscope properties of the flakes in the isotropic and nematic phases. The GO exhibited different dielectric relaxation modes in different media. In addition, the smaller flakes exhibited a faster relaxation as compared to the larger flakes. There are several factors that can affect the dielectric behaviour of GO flakes suspensions: the dielectric constant and the viscosity of the host medium, and the concentration and alignment direction of GO. Figure 1 shows the relative permittivity of GO in isopropanol and in the nematic material (5CB) for different temperatures. The observed relaxation behaviour will be discussed.

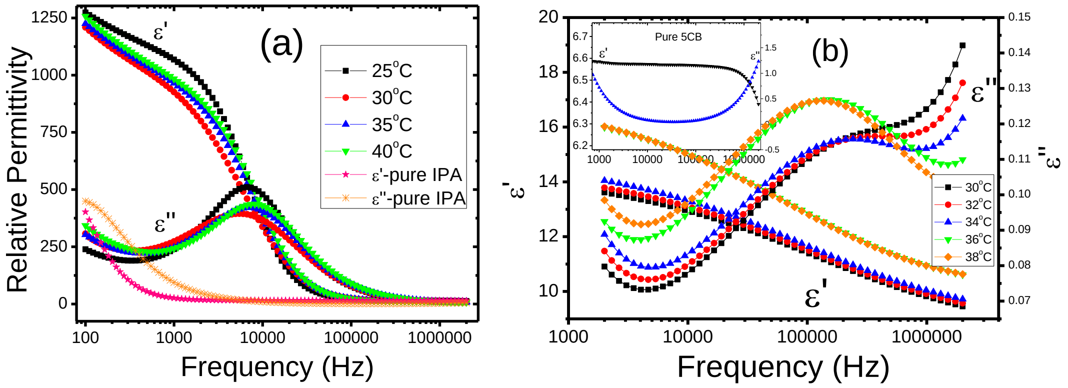

Figure 1. The real and the imaginary part of the relative permittivity as a function of frequency at 0.1 AC volts for a range of temperature for GO (≈0.5µm in diameter) in (a) isopropanol (IPA) (b) 5CB.

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On zero rotational diffusion constants in nematics

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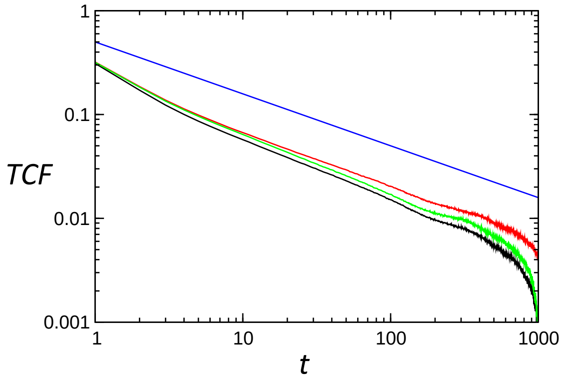
It is commonly assumed that the time taken for a molecule to significantly change its orientation is roughly the inverse of its rotational diffusion constant, D_r. If, for simplicity, we focus on axially symmetric particles, such as a rod or a disc, then in an isotropic fluid, one has the result:

$$1/D_r = l(l+1)\int_0^\infty \left\langle C_m^l\left[\hat{\mathbf{u}}(t)\right]C_m^{l*}\left[\hat{\mathbf{u}}(0)\right]\right\rangle dt \qquad (1)$$

Here $\hat{\mathbf{u}}(t)$ is the unit vector along the molecule's symmetry axis at a time t, and C_m^l is an unnormalised spherical harmonic. The angled brackets indicate a time-correlation function (*TCF*).
To see if a similar result holds in the nematic phase, we have conducted molecular dynamics simulation studies of a system of Gay-Berne particles [1] and have calculated $\left\langle C_m^2\left[\hat{\mathbf{u}}(t)\right]C_m^{2*}\left[\hat{\mathbf{u}}(0)\right]\right\rangle$. Of particular interest is the value of this correlation function when m = 1. The plot is shown below:



The scales are logarithmic. The three lower curves are simulation results while the top, blue curve is a straight line of gradient -1/2. We conclude that, at long times, the correlation function has an asymptotic power law dependence, proportional to $-1/\sqrt{t}$. In that case eq. (1) yields a zero rotational diffusion constant, as the integral of the TCF is infinite.

This long-time behaviour has been predicted previously by theory [2] and there is NMR evidence for such behaviour in a nematic [3], but to our knowledge, this is the first time this effect has been seen using computer simulation.

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NIR Kerr effect in polymer-stabilized blue phase liquid crystals

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Polymer-dispersed blue phases are promising candidates for a new generation of liquid crystal (LC) displays. Blue phases (BPs) *[1]* are chiral mesophases, which have been mainly studied in calamitic thermotropic LCs. Owing to a cubic superstructure of the local molecular alignment, BPs are optically isotropic but can show a very large electric field-induced birefringence. The present contribution is focused on studying the electric field-induced birefringence in the near infrared (NIR) spectral range. The Kerr coefficients observed in the NIR range, $K \approx 0.6 \cdot 10^{-9}$ m V^{-2}, are slightly smaller than the values in the visible range, $K \approx 10^{-9}$ m V^{-2} *[2]*, which can be explained by the dispersion of the refractive indices. Nevertheless, the results indicate promising features for optical communication and other NIR applications.

Apart from practical aspects, our observations show a two-step mechanism of the field induced transformation. For moderate voltages, the induced birefringence Δn is described by the electrooptic Kerr effect, $\Delta n = K \lambda E^2$, where λ is the wavelength of the light and K is the Kerr coefficient. In order to describe that the field-induced birefringence Δn reaches a saturation value Δn_S at high field strength $E \approx E_S$, Wu and co-workers *[3]* have proposed an extended Kerr model, where the field-induced birefringence is described by the equation $\Delta n = \Delta n_S \{1 - \exp[-(E/E_S)^2]\}$. In addition, our experimental data $\Delta n(E^2)$ show a discontinuous change and a hysteresis at intermediate voltages (Figure 1). The behaviour for larger field strengths is well described by the equation $\Delta n = \Delta n_S \{1 - \exp[-(E-E_1)^2/(E_S-E_1)^2]\}$, where E_1 is an electric field that is related to the kink of the $\Delta n(E^2)$ curves.

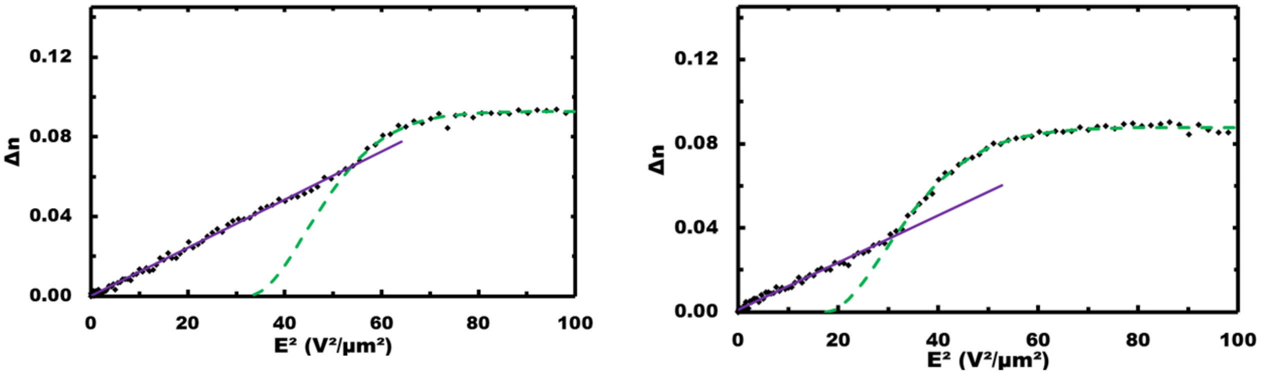

Figure 1. Field-induced birefringence on (left) increasing voltage and (right) decreasing voltage, respectively.

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Lyotropic liquid crystalline templated synthesis of silver nanoparticles

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Metal nanoparticles have attracted a lot of attention in the field of colloidal and material science due to their unique electronic and optical properties. Because of the broad field of potential applications there is also a growing interest in developing new green methods for the controlled synthesis of the nanomaterials. Due to the rich polymorphism, lyotropic liquid crystals formed by amphiphilic molecules are particularly interesting templates to control size and morphology of nanoparticles.

In this contribution we report the synthesis of silver nanoparticles in the various lyotropic liquid crystalline phases formed by biologically friendly surfactants with or without cationic surfactant-DNA complexes in aqueous solution with different additives [1-2]. Two different preparative strategies have been applied. Firstly, surfactant molecules have been used to form the liquid crystalline phases in aqueous solution as well as to reduce the silver ions into silver atoms as confirmed by FTIR and ^{1}H NMR spectroscopy. Secondly, by using DNA-containing liquid crystals silver nanoparticles were synthesised via photoreduction of the DNA-Ag^+ complexes where the DNA itself may act as template [3].

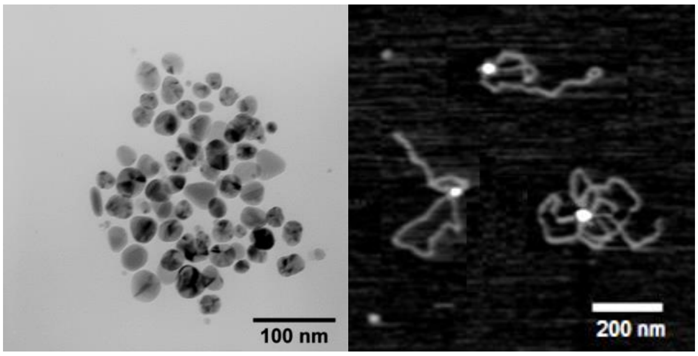

Figure 1. (Left) TEM image of synthesised nanoparticles, (right) AFM image of the extracted DNA

The effect of the formation of silver nanoparticles on the lyotropic liquid crystalline phase was investigated with small angle X-ray scattering, polarising optical microscopy and ^{2}H NMR spectroscopy. On the other hand, the influence of the template mesophase (which may or may not contain DNA) on the formation rate and nanoparticle size and morphology is studied using UV-spectroscopy, TEM and AFM.

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Surface grafted crosslinker in polymer network liquid crystals

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Surface grafted benzophenone silane (4-(3-chlorodimethylsilyl)propyloxybenzophenoe, BPS) *[1]* was used as novel kind of photo initiator to generate polymer network liquid crystals (PNLCs). BPS was synthesised and successfully immobilised on the surfaces of ITO-glass plates. Subsequently, the coated substrates were used to assemble LC test cells. To generate a PNLC, E7 was used as host LC, which was doped with two different kinds of reactive mesogens (BAB6 and RM257), respectively. Capacitance measurements during UV exposure of the LC test cells were carried out and turned out to be a straightforward method to detect changes in the dielectric properties of the LC. In a systematic study, the electro-optic response times were detected in a complete set of samples before and after UV curing of the reactive mesogens. These experiments clearly showed the ability of surface grafted BPS to initiate photopolymerisation in the doped host LC. The combination of BPS with a conventional photo initiator yielded a reduction of the electro-optic decay times (Figure 1) of 30% – 50% as compared to PNLCs formed with only a conventional photo initiator.

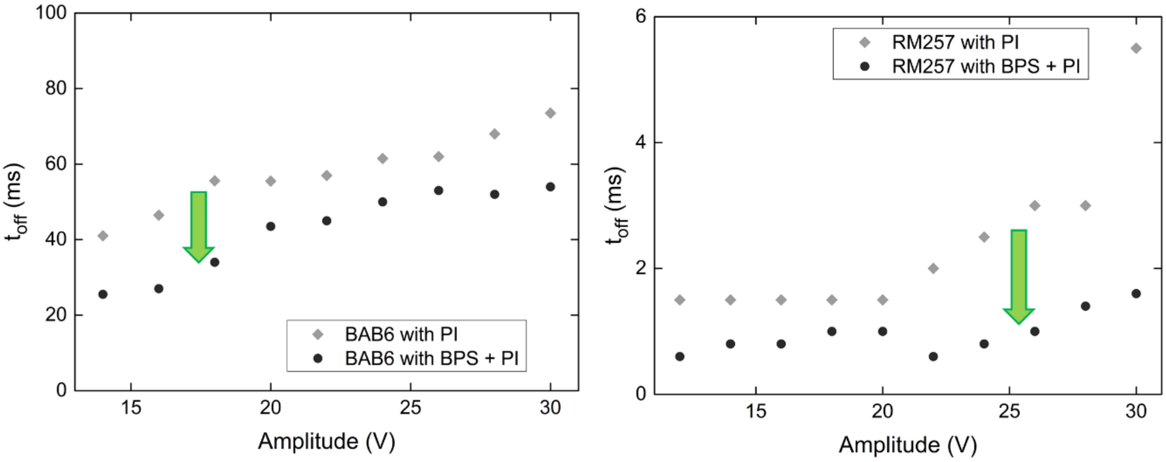

Figure 1: Decay times for BAB6 (right) and RM257 (left) with and without BPS after UV curing.

A possible reason for the enhanced response times is a reduced bundles radius of the formed polymer network *[2]*. PNLCs with enhanced electro-optical properties have high potential for various photonic applications *[2-5]* based on swift continuous phase modulation. The measured data show that use of surface grafted photo initiators is very promising to further push the response times in PNLCs and enhance their electro-optic properties because in a BPS-initiated PNLC the decay times were up to 50% faster than without BPS.

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Electrooptics of blue phase photonic crystal fibres

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Liquid crystalline blue phases (BPs) are promising mesophases for photonic applications due to their continuous electrical tuning and their fast response times. In contrast to many other liquid crystals, BPs do not require an alignment layer *[1]*. In general, the BPs are isotropic, but an external electric field induces birefringence. The latter is proportional to the electric field squared like in a Kerr medium. These properties make BPs also interesting for the use in photonic crystal fibres (PCFs). PCFs typically consist of a hexagonal array of air inclusions surrounding a solid glass core [Figure 1(a)]. Light is confined to the core by the photonic properties of the cladding.

We infiltrate the inclusions of a PCF (LMA10 from NKT Photonics) with a blue phase mixture (97.2% liquid crystal host MDA-PB-3 with 2.8% chiral dopant R5011, both from Merck [Fig. 1(b)]), which leads to a photonic band gap fibre with the typical spectral transmission windows [Fig. 1(c)]. Their positions depend on the refractive index of the infiltrating blue phase *[2]*.

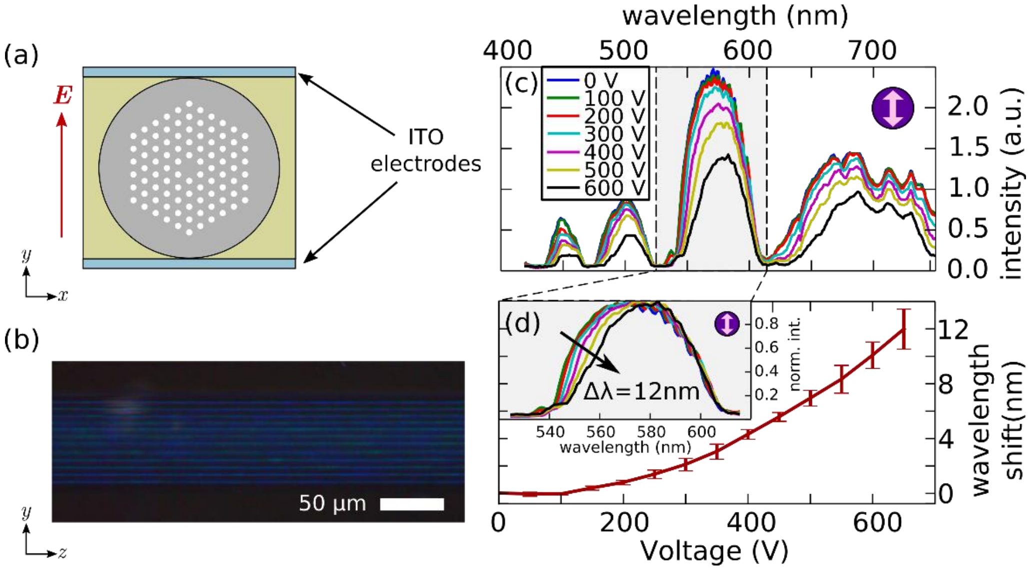

Figure 1. (a) Schematic of a PCF sandwiched between ITO electrodes. (b) Microscope image in reflection of a blue phase in a PCF at 66.0°C. (c) Transmission spectrum of light coupled into the blue phase PCF for different voltages. (d) Voltage dependent shift of the left edge of the transmission window between 520 and 620 nm. The inset shows the corresponding normalised intensity.

Applying an external voltage induces a birefringence that shifts the transmission windows [Figure 1(c)] to longer wavelengths if the polarization coincides with the direction of the external electric field. Evaluation of the shift shows a quadratic dependence on the applied voltage [Figure 1(d)] as expected from the Kerr effect. This effect can be used to determine the Kerr constant with help of the ARROW model [3].

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Pattern formation and inverse dynamic light scattering in a liquid crystal with negative and positive anisotropy of electric conductivity

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The appearance of regular patterns or chaotic turbulence based on electroconvection (EC) was one of the first electro-optical effects observed in liquid crystals. EC refers to the occurrence of mechanical flow due to an electric current. An example of EC is the formation of Williams domains (Figure 1) *[1].* The latter were first observed in liquid crystals with negative dielectric anisotropy $\Delta\varepsilon$ and positive conductivity anisotropy $\Delta\sigma$, so-called (-,+) materials *[2],* and explained by the Carr-Helfrich mechanism (standard-EC, s-EC) *[3, 4].* Later, EC was also observed for (+,-) materials [$\Delta\varepsilon > 0$, $\Delta\sigma < 0$] and found to be describable by the standard model, as well *[3, 4].* While s-EC is not expected for (-,-) or (+,+) materials *[2-4],* the latter show also electroconvection, but exhibit different patterns (non-standard EC, ns-EC) *[5, 6].*

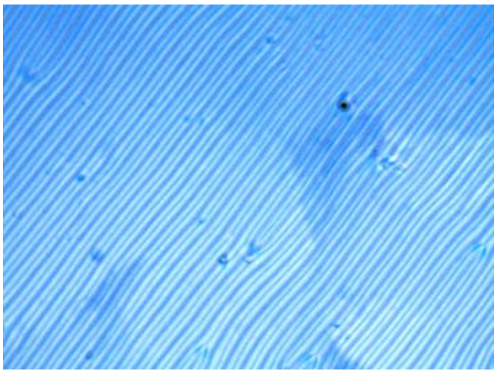

Figure 1. Williams domains in a 10 µm thick sample of 95% HEXOAB and 5% 7OCB with 0.001% TOAB.

Here, we present studies of EC in the very interesting case, where a nematic liquid crystal shows a temperature-induced transition of the signs of $\Delta\varepsilon$ and $\Delta\sigma$ from (+,-) to (+,+). Such materials were described long ago by Heppke and coworkers *[7]*. They were found to show an “inverse” light scattering effect but have not been studied in great detail *[8]*. Here, we restrict ourselves to the conduction regime and describe the appearance of different patterns in samples with both homeotropic and planar anchoring. The correlation between frequency and threshold voltage is also investigated.

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New aryl end-capped bent-shaped liquid crystals

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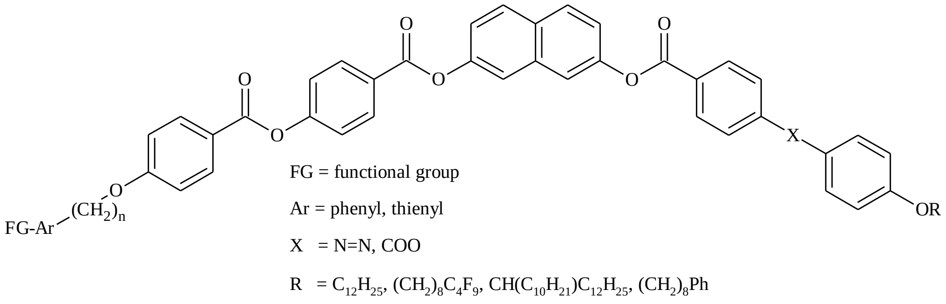
After the discovery of polar macroscopically chiral mesophases formed by achiral bent-core molecules in 1990´s *[1]*, numerous bent-shaped mesogens were prepared and studied in order to recognize structure-property relationship. To tune mesomorphic properties of the materials, various approaches, such as changing the character and orientation of the linkages, introducing lateral substitution or varying the length of terminal alkyl chains, can be applied. General requirements for the design of bent-core materials and the results of investigation of mesomorphic behaviour were summarized in numerous reviews *[2,3]*.

The presented work is focused on the design and synthesis of aryl terminated bent-shaped molecules (Figure 1). Naphtalene-2,7-diol was used as a central core, phenyl and thienyl were introduced in the terminal position of a lengthening arm. Within the series of thienyl end-capped materials, the influence of the type of the linkage and terminal alkyl chain on mesomorphic properties was investigated. Within the series of phenyl end-capped materials, not only the influence of the linkage and type of terminal alkyl chain on their mesomorphic behaviour was investigated, but also the impact of the length of phenylalkyl chain and the influence of exchange of one methylene unit by oxygen were studied. Terminal aryl moiety will be functionalised and these materials will be used as ligands to decorate nanoparticles to obtain a new kind of hybrid materials.



FG = functional group
Ar = phenyl, thienyl
X = N=N, COO
R = $C_{12}H_{25}$, $(CH_2)_8C_4F_9$, $CH(C_{10}H_{21})C_{12}H_{25}$, $(CH_2)_8Ph$

Figure 1. General structure of synthesized liquid crystals

Mesomorphic properties of prepared liquid crystals were investigated by optical polarising microscopy, differential scanning calorimetry and x-ray spectroscopy.

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Chiral isotropic liquid and bicontinuous cubic phases in achiral polycatenar LC molecules

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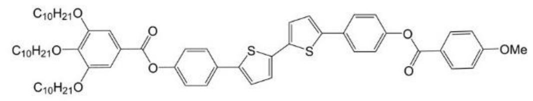
Recently, intriguing dynamic mirror symmetry breaking phenomena have been reported in the isotropic liquid *[1]*, as well as in bicontinuous cubic phases consisting of infinite interpenetrating networks *[2]* formed by achiral polycatenar liquid crystalline compounds. Here we report the observation of chiral isotropic liquids formed by a series of achiral polycatenar rod-like molecules, and also the transition from chiral liquids to achiral bicontinuous $Ia\overline{3}d$ cubic phase. Compound **1** represents one of these polycatenar molecules based on a 5,5'-diphenylbithiophene core. According to small angle X-ray scattering (SAXS) results, on cooling of compound **1** from isotropic liquid, it transforms to the cubic $Ia\overline{3}d$ phase at 168 °C. Synchrotron circular dichroism (SRCD) spectra, on the other hand, show strong CD signals appear in the temperature range between 193 °C and 180 °C (see Figure), before they disappear on transition to the $Ia\overline{3}d$ phase. This indicates that a chiral isotropic phase is formed, prior to the formation of the cubic phase, from the ordinary achiral isotropic liquid phase. This is also confirmed by the presence of a DSC peak showing an exotherm at the first order liquid-liquid transition on cooling at 192 °C.



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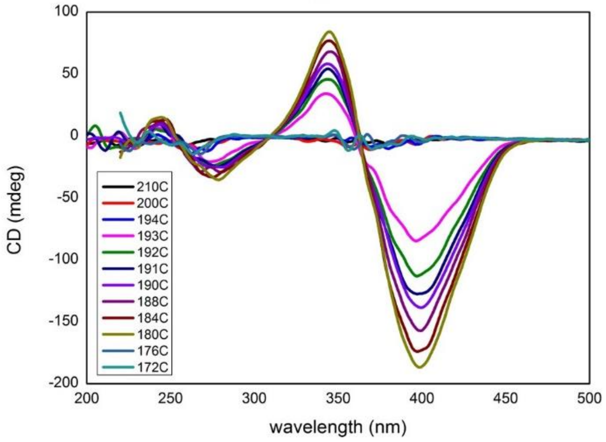

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A c2mm liquid crystal phase formed by dimer molecules

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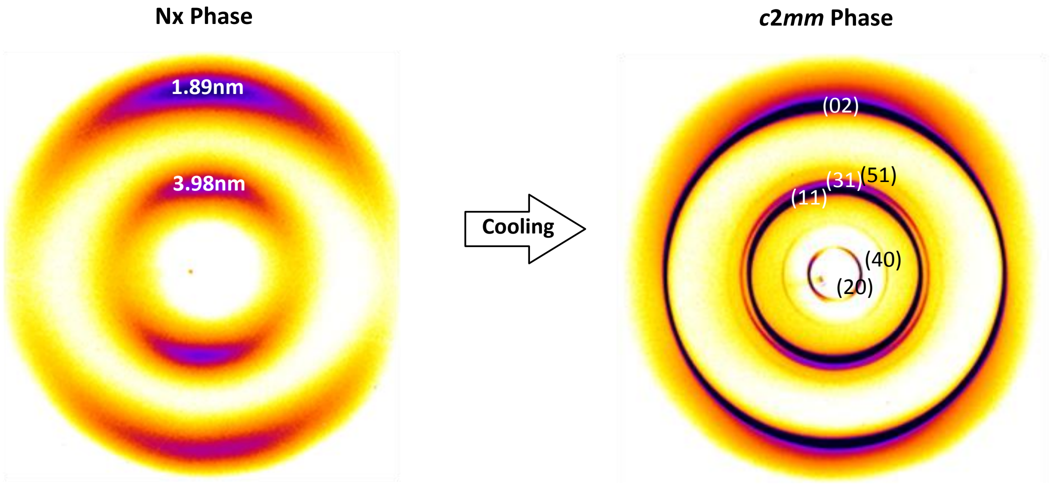
In recent years the nematic – nematic transition observed in LC dimers with an odd spacer has attracted significant attention. The theorised existence of helical chirality within the lower temperature nematic, often termed the Nx or Ntb phase, has been the primary focus of investigation *[1,2]*. To date the proposed conical helices continue to elude unambiguous identification through conventional characterisation techniques; as such we turn our attention to the liquid crystal (LC) phases formed below the Nx. Here we present a modulated smectic c2mm LC phase formed upon cooling the Nx phase of DTC7C5 through a first order phase transition. This phase was characterised through grazing incidence and transmission X-ray scattering experiments which reveal a centred rectangular unit cell (spacegroup c2mm) with lattice parameters 'a' = 27.21 ± 0.07nm (modulation wavelength) and 'b' = 4.145 ± 0.007nm (layer spacing). We explain the periodic shift in the molecular arrangement using a model similar to that provided in explanation of the B1 banana phase of polar bent core mesogens *[3,4]*. However in contrast to the B1 phase, the step does not create layer discontinuity, but instead produces interlocked double layers. The (11) and (02) lattice spacing of these double layers were found to respectively coincide with the ~1.9 and ~4nm scattering maxima observed within the Nx phase. This, as well as the similarity in POM textures, may suggest that the two phases are in fact closely related. This work may therefore bring us a step closer to determining the true structure of Nx phase.



Nx Phase

***c2mm* Phase**

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Helfrich-Hurault effect in smectic A (SmA)

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We consider a refined analysis of the Helfrich-Hurault (H-H) effect in SmA when the layer normal $\vec{a}$ and the director $\vec{n}$ are decoupled. We demonstrate that the H-H transition threshold decreases as $\vec{a}$ and $\vec{n}$ decouple. The dependence of this transition upon the compression coefficient B_0 is discussed. For example, the wave number behaviour dependence on the electric field magnitude, the elastic coefficient dependence and the critical range values for B_0 -which gives the most sensitivity to the electric field dependence.

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Deuterium isotope effect on the stability of the lyotropic $L_{\alpha'}^*$ phase

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With our resent discovery of the lyotropic analogue to the chiral ferroelectric smectic C (SmC*) phase ($L_{\alpha'}^*$ phase in lyotropic terminology) *[1]*, the important question emerges, how the tilt directions of the amphiphile bilayers are long-range correlated across the solvent layers in between consecutive bilayers, such that the director becomes macroscopically tilted to the layer normal. Previous investigations indicated that the strength and the density of the hydrogen bond network inside the solvent layers play a crucial role in this tilt correlation mechanism *[2]*.

To gain further insights into the role of the hydrogen bond network, we now investigate whether or not the deuteration of the hydrogen bonds affects the stability and the properties of the tilted $L_{\alpha'}^*$ phase. Figure 1a shows the phase diagram of our chiral amphiphile ((*R*)-3-(2-(4-(5-heptylpyrimidin-2-yl)phenoxy)ethoxy)propane-1,2-diol) with formamide (FA). Using deuterated formamide (d-FA), the phase diagram (Fig. 1b) is significantly changed, even though the densities of the hydrogen bond networks are essentially the same in FA and d-FA. In particular, the stability of the tilted $L_{\alpha'}^*$ phase is considerably reduced in comparison to Fig. 1a. Furthermore, optical tilt angle measurements show that in mixtures with d-FA the saturated $L_{\alpha'}^*$ tilt is reduced by 15 – 20% in comparison to the non-deuterated mixture with same molar composition.

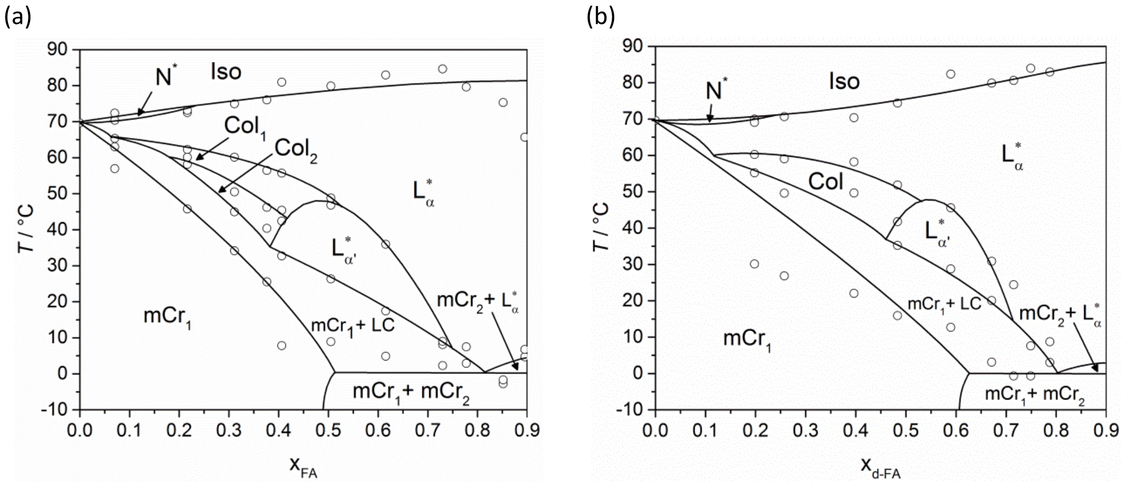

Figure 1. (a) Phase diagram of formamide/Diol system and (b) phase diagram of deuterated formamide/Diol system.

The substitution of hydrogen by deuterium mainly reduces the frequency of the hydrogen bond vibration and, thereby, changes the collective dynamics of the hydrogen bond network. The clear isotope effect on the stability of the $L_{\alpha'}^*$ phase thus indicates that not only the strength and the density of the hydrogen bond network but also its dynamics is important for the tilt correlation mechanism leading to the macroscopic director tilt in the lyotropic $L_{\alpha'}^*$ phase.

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Nanosegregation and its connection to “de Vries-like” properties in smectic liquid crystals

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In smectic A (SmA) to smectic C (SmC) transitions of the “de Vries”-type, the appearance of director tilt is coupled to a substantial increase in optical birefringence and thus in orientational order, the increase of which – more or less – compensates the smectic layer contraction in the SmC phase [1]. This mechanism however basically requires SmA phases with unusually low orientational order and rather high smectic order. A promising route towards “de Vries-like” smectics is thus the incorporation of nanosegregating segments such as terminal siloxane or carbosilane groups into the mesogens [2]. In these materials the direct isotropic to SmA transition is essentially driven by nanosegregation even though their orientational order remains low. The high translational order in SmA phases of carbosilane-terminated mesogens was proven by freeze fracture TEM images.

We recently reported on a new chiral smectic liquid crystal QL32-6 undergoing a SmA* – SmC* transition with maximum layer contraction of only 0.2% [3]. We have now investigated a series of similar mesogens (cf. Fig. 1a) all having a SmA* – SmC* phase sequence but with terminal carbosilane segments of different length to systematically study the influence of nanosegregation. The phase sequences and smectic layer spacings as well as the optical birefringences (Fig 1b) and tilt angles are studied and discussed with respect to the SmA* – SmC* phase transition and its “de Vries-like” properties. All findings consistently show that the manifestation of “de Vries-like” behavior crucially depends on the nanosegregating subunit. This is most relevant for the rational design of new “de Vries”-type materials.

The authors gratefully acknowledge financial support from the Deutsche Forschungsgemeinschaft (DFG) and the National Science and Engineering Council of Canada.

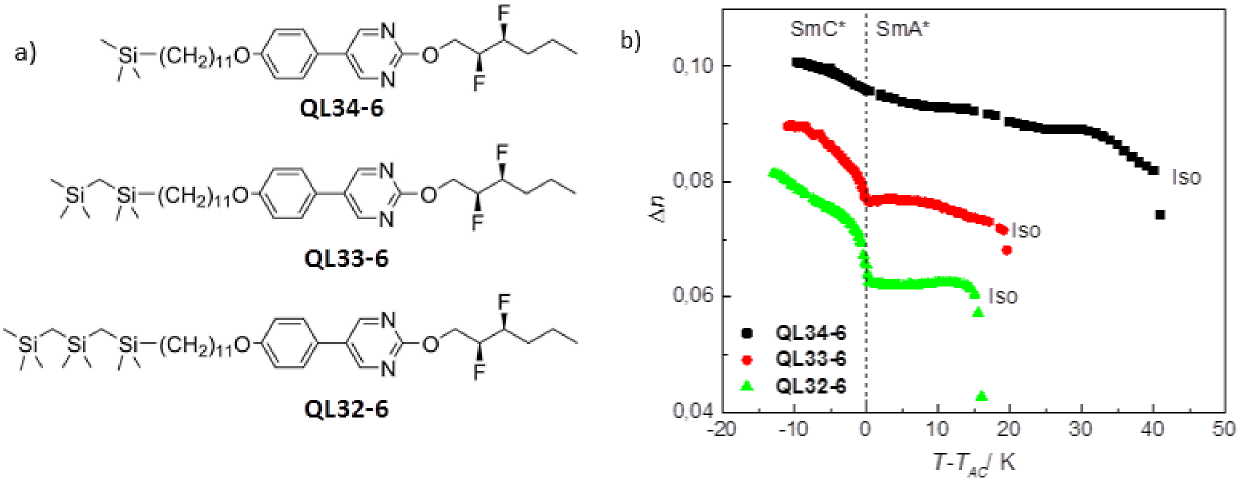

Figure 1. a) Chemical structures of the investigated smectic compounds and b) temperature dependent birefringence $\Delta n(T\text{-}T_{AC})$ of the three nanosegregating liquid crystals.

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Electro-optic Kerr effect in ionic liquid crystals

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The electro-optic Kerr effect, which was first observed by John Kerr in 1875, is a quadratic electro-optic effect inherent to all states of matter and related to the molecular orientational order induced by an electric field E. Kerr observed a quadratic dependence between the induced optical birefringence Δn and E:

$$\Delta n(\lambda, E) = B \lambda E^2$$

where B denotes the temperature-dependent Kerr constant and λ the wavelength of light. For nematic liquid crystals such as 5CB (with $B = 12.41 \cdot 10^{-11}$ mV^{-2} at $T - T_{NI} = 0.17$ K *[1]*) an exceptionally large Kerr effect was found in the pre-transitional regime from the isotropic to the nematic liquid crystalline phase.

Ionic liquid crystals (ILCs) are very interesting for Kerr effect studies because of their ionic character which makes them highly polar mesogens. To avoid complications with ionic conductivity a high frequency AC field was applied and an ILC (Fig. 1a) with low clearing temperature (71.4°C) and a bulky counter-ion was chosen. An example of its electro-optic Kerr-response in the isotropic phase is seen in Fig. 1b. In this contribution we present first systematic results of Kerr effect measurements on this ILC, namely the dependence of the Kerr effect on the temperature and the electric field strength. At high field strength we observe systematic deviations from Kerr's law, which have also been reported for other ionic systems such as micellar solutions of ionic amphiphiles *[3]*.

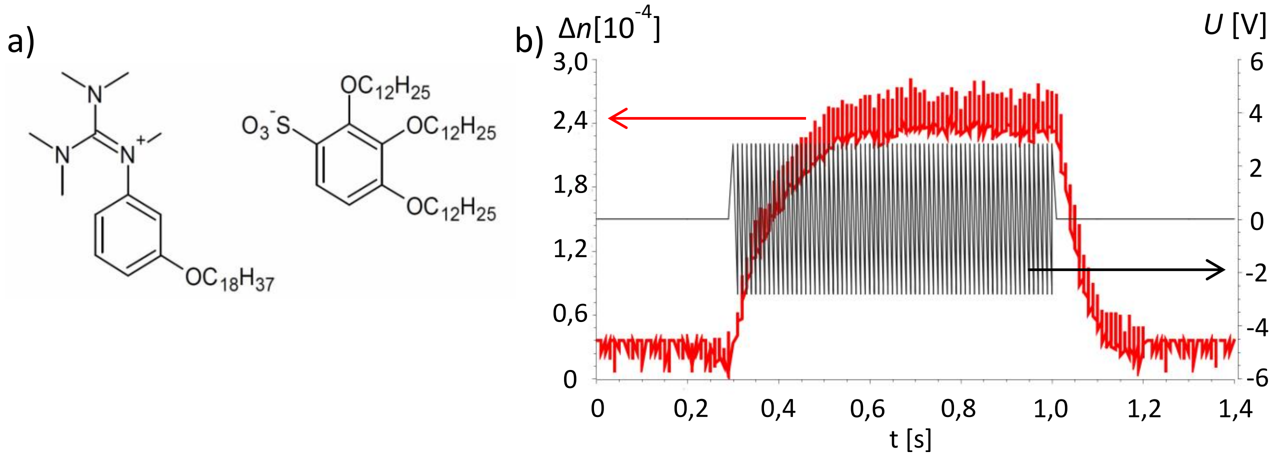

Figure 1: a) Molecular structure of the ILC *[2]* and b) its time resolved electro-optic Kerr response 0,6 K above the clearing temperature on application of a 1kHz square wave voltage; electrode gap: 20µm.

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Investigation of electronic charge transport properties in liquid crystals with higher ordered smectic phases

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Since the 1990s discotic liquid crystals with columnar phases have been known as one dimensional organic semiconductors. However, electronic charge transport in smectic phases of rod-like mesogens has been investigated far less. Due to the layered structure, charge carriers can in principle easily diffuse in two dimensions along the smectic layers and the charge transport is thus expected to be less sensitive to structural defects than the 1D transport in columnar phases. Since the molecular order and the packing density inside the smectic layers is high, mainly higher ordered smectic phases are considered as potential 2D semiconducting materials. So far electronic charge transport has only been studied in detail for a few examples of terthiophene-, 2-phenylbenzothiazol- and 2-phenylnaphthalene-derivatives *[1,2]*.

To get deeper insight into the 2D electronic charge transport in higher ordered smectics, we selected two mesogens with similar dimensions but different electronic structures of their mesogenic cores (Figure 1a). The terthiophene **1** shows only tilted liquid crystalline SmC, SmF and G phases *[3]*, whereas the terphenyl **2** has three different higher ordered smectic phases, one of which is orthogonal ($\mathrm{SmB_{hex}}$). The intra-layer order of the smectic phases was investigated by X-ray diffraction and the charge transport was studied with a field effect transistor setup (FET, Figure 1b) in order to understand the correlations between the electronic core structure of the mesogen, the molecular packing in the smectic phases and the charge carrier mobility. Even though the intra-layer correlations were found to be rather similar for the two compounds, charge transport measurements confirmed a significantly higher mobility for terthiophene **1**. These results indicate that the unoccupied d orbitals of the sulphur heteroatoms are essential for effective charge transport mechanisms. The mobilities found for the two higher ordered phases SmF and G (10^{-3} cm² V^{-1} s^{-1}) are in the range between the crystalline phase ($3 \cdot 10^{-2}$ cm² V^{-1} s^{-1}) and the fluid SmC phase ($5 \cdot 10^{-4}$ cm² V^{-1} s^{-1}).

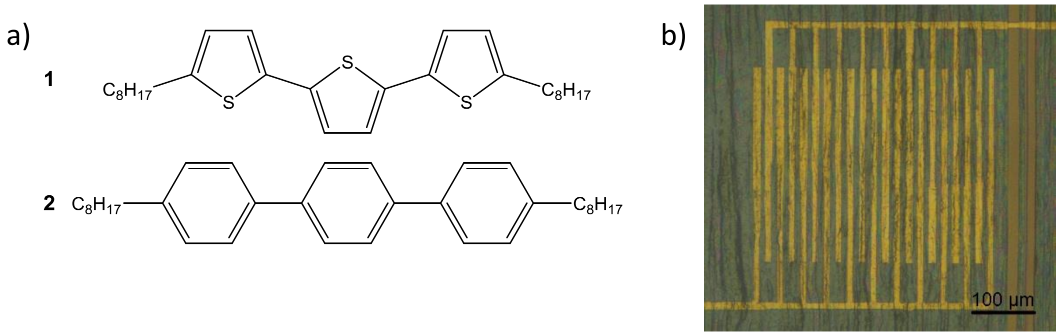

Figure 1. a) Chemical structures of the investigated smectic compounds and b) transistor substrate with an aligned film of compound **1** prepared by mechanical shearing.

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Design and evaluation of tunable microwave electric-LC resonators based on liquid crystal

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Liquid crystals have suitable properties to be used for tuneable devices at microwave frequencies. In this research, due to the anisotropic properties of liquid crystals in their nematic phase, voltage-controlled tuneable ELC resonators are proposed to achieve large tuning range.

Three different ELC resonators are designed and optimized to get the maximum tuneability. The original ELC resonator, as shown in Figure1(a), consists of inductive loops and a capacitive gap *[1]* and uses liquid crystals to sweep the resonance frequency. The original ELC resonator is optimized to have a result of a maximum frequency tuning of 6% with using the liquid crystal Merck E7.

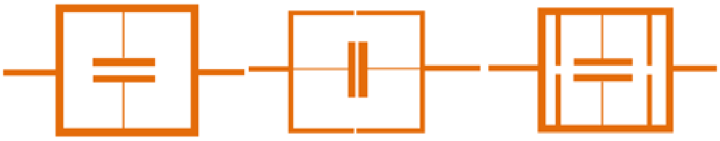

Figure 1. (a) Original structure (b) Amended structure (c) New structure

The original structure is amended and re-designed, compared with the original structure, the new design adds two gaps of the inductive loops (Figure 1(b)), and the results show that the tuneability has increased from 6% to 7%. Moreover, a new ELC resonator is proposed and shown in Figure 1(c), which adds two inductive loops with gaps. The modelled results show that the resonance frequency shifts from 6.89GHz to 6GHz, which has the tuning range of 890MHz, as can be seen from Figure 2, and the tuneability of this structure is 14%. The structure is being fabricated for testing.

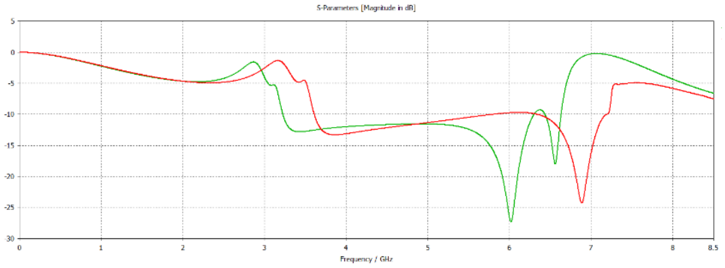

Figure 2. The S11 parameters of new ELC resonator

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Instabilities and phase behaviour of active liquid crystal droplets

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We consider a continuum model of the cell cytoskeleton as an active liquid crystal where the constituent particles are driven out of equilibrium by consumption of chemical energy (based on *[1,2]*). We predict, analytically and numerically, a variety of spontaneous symmetry breaking behaviour driven by activity when this material is confined to or on fluid droplets immersed in a passive fluid.

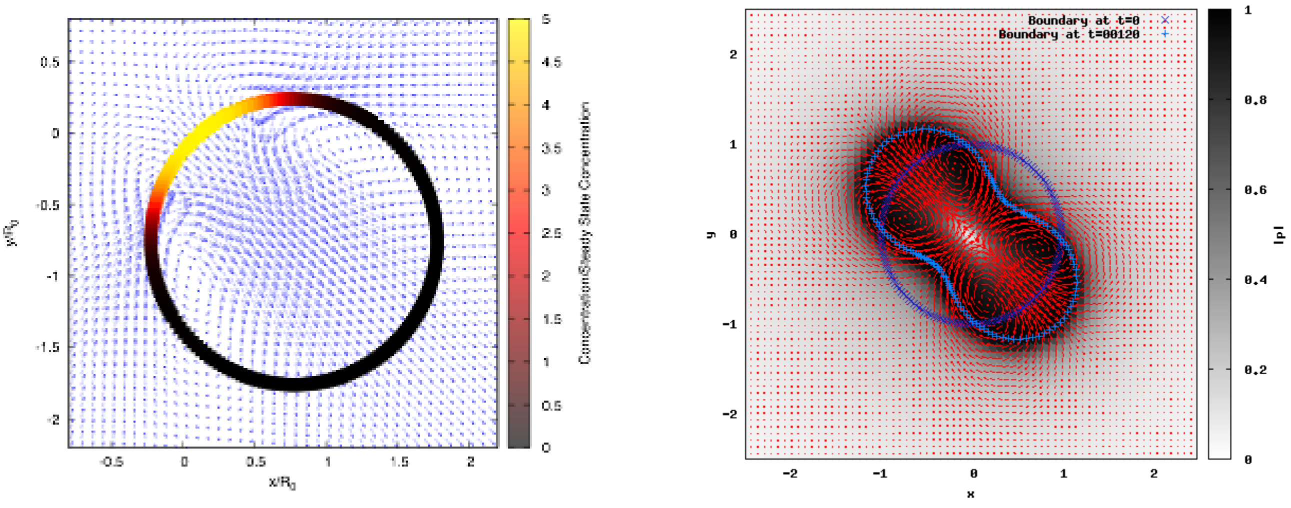

Figure 1. Snapshots of our active droplet simulations. *Left:* A fluid droplet with an active contractile fluid dispersed on the interface in a steady swimming state. The solid line shows the interface, with colour showing the concentration density of active fluid and the blue arrows indicating the flow. *Right:* A droplet of active polar matter deforming due to contractile activity. The shading shows the polarisation magnitude with a defect at the droplet centre and the red arrows show the flow field. The dark and light blue lines show the initial and current positions of the droplet interface respectively.

These activity driven instabilities can lead to rich phase behaviour of the droplets including steady state motility, deformation, and oscillations *[3]*. I will discuss how these states may be observed experimentally in vitro using reconstituted cytoskeletal networks and also the limitations of this model. Finally, I will demonstrate ways this model can be improved in the future to closer represent a model of cytoskeleton driven motility and deformation in animal cells.

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LC tweezers – filled tetrasubstituted star-like liquid crystal materials

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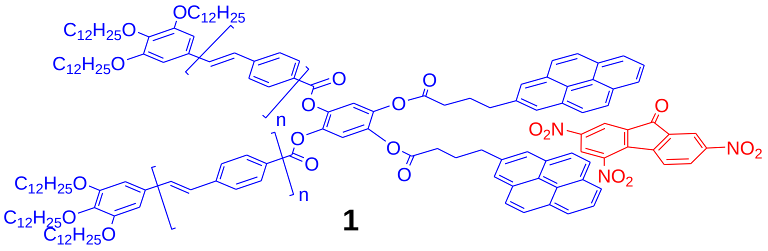
Star-shaped mesogens have been explored for a wide range of molecular motifs *[1]*. The arm building blocks can be flexible, semi-flexible or shape-persistent. When mesogens are attached via a flexible spacer to a 1,3,5-trisubstituted benzene, the mesogens self-organise in conventional LC assemblies. In contrast, the semi-flexible oligobenzoate arms are folding to conformers of various shapes. In the latter case the whole conformer is the new mesogen organising in lamellar, columnar or cubic LC phases. Tetrasubstituted benzene mesogens, for which the arms are attached in 1,2- and 4,5-positions should arrange the arm building blocks side by side *[2]*. Based on this structural design, molecule **1** was envisaged as a promesogen, which might interact with molecules or particles possessing a large π-surfaces in order to solubilise them in liquid crystal structures.



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Here we will present the synthesis of the title compounds, the aggregation in solution the thermotropic properties of the neat material as well as the mesophase behaviour of mixtures with trinitrofluorenone (TNF) by polarised optical microscopy and differential scanning calorimetry. It will be shown that the pyrene binds selectively the electron-deficient TNF like a tweezer and stabilises the liquid crystal phases. The structure of the nanotweezer LC assemblies is studied by X-ray scattering, modelling and fibre diffraction simulation.

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The stabilisation of smectic mesophases by bulky end groups

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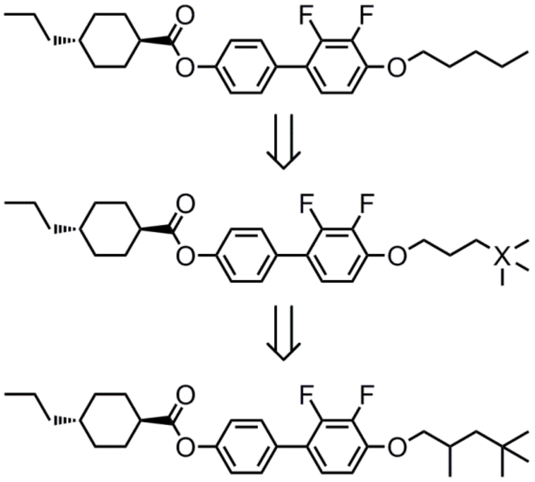
The ability to exert control over the bulk thermal properties and polymorphism of a liquid crystalline material through rational design of its molecular structure is a cornerstone of the liquid crystal display industry. Commercialisation of ferroelectric LCDs has proved difficult for many reasons, one of which is a need for better materials with higher thermal stability of the smectic C phase whilst retaining the N-SmA-SmC phase sequence.



Cr 85.8 (SmC 75.1) N 179.2 I

X = C: Cr 105.0 SmC 108.7 N 139.3 I
X = Si: Cr 84.9 SmC 103.4 SmA 105.6 N 124.5 I

Cr 55.8 SmC 68.7 SmA 88.4 N 103.0 I

Figure 1

Admittedly, the materials in this poster are unlikely to be of any real-world use for devices. However, the 4-alkoxy-2,3,difluorobiphenyl 4-alkylcyclohexyl carboxylate system is trivial to prepare synthetically, and serves as something of a testbed, and by preparing a range of materials we can attribute changes in bulk properties to specific changes in molecular structure. Starting from a simple system bearing two linear terminal aliphatic chains we have prepared several families of materials incorporating bulky end groups. The incorporation of *tert*-butyl (^{t}Bu) or trimethylsilyl (TMS) units as end groups leads to dramatic increases in the thermal stability of smectic mesophases at the cost of significantly reduced clearing point. Moving to bulky groups with a larger steric footprint (2,4,4-trimethylpentyl) this stability of the smectic C phase is diminished relative to the parent material, whereas it is enhanced for the smectic A phase. We present an investigation into the properties of these materials using POM, DSC and SAXS.

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The mesomorphic behaviour of unsymmetrical methylene linked phenylbenzoate dimers

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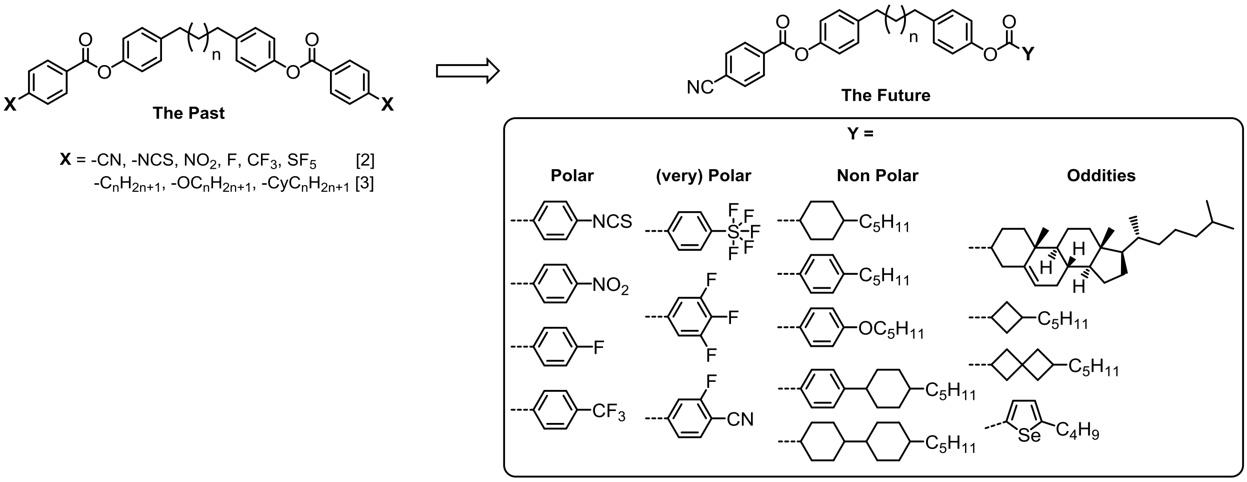
Efforts to understand the structure and properties of the twist bend nematic phase – NTB or NX depending on the viewpoint of the reader - continue to motivate the synthesis and characterisation of novel liquid crystal bimesogens *[1]*. Building upon our previous work on symmetrical liquid crystal dimers *[2,3]* we have recently forayed into unsymmetrical bimesogens. The choice of phenyl benzoate mesogenic units permits rapid synthesis and purification, whilst a diverse array of materials can be prepared from suitable benzoic/carboxylic acids many of which are available commercially. More exotic carboxylic acids such as trans 2-alkylcyclobutyl, trans, trans 2′-alkylbicyclobutyl, cholesteryl and 2-butylselenophene were available to us in house.

The nematic and NTB phases were exhibited by all unsymmetrical bimesogens with two 'polar' mesogenic units. We find that certain combinations of polar/non polar mesogenic units give rise to an additional nematic-like mesophase below the NTB phase, providing fresh impetus to study unsymmetrical dimeric systems. The ability to incorporate functional groups that are typically detrimental to mesophase stability (such as SF5) raises the possibility of incorporating specific molecular features to aid spectroscopic study of mesophase structure.



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Control of the bend angle in dimers allows manipulation of the stabilities of the nematic and twist-bend mesophases

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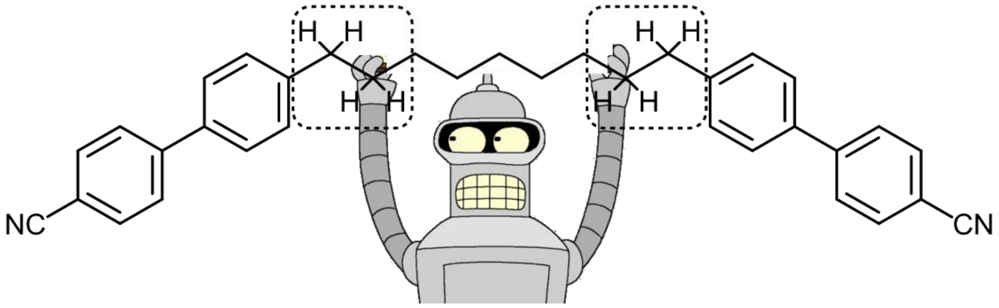
Over recent years dimeric liquid crystals have been found to exhibit a variety of fascinating mesomorphic properties. Bimesogens which have a spacer of odd parity have been found to exhibit a transition from a nematic phase to a lower-temperature mesophase that has been classified as the twist-bend nematic phase (NTB) *[1-5]*.

Methylene linked dimers such as CB9CB have received extensive study due to their propensity to exhibit the NTB phase *[2,3]*. In this study the incorporation of other linking groups (imines, ethers, alkynes, esters etc.) in lieu of the methylene-linking group has allowed us to study the relationship between the gross molecular bend and the twist-bend nematic phase.



Chemically bonded methylene units cannot, unfortunately, simply be chopped out and replaced. However, we can synthesize analogues of CB9CB with varied linking groups, whilst and a combined approach using DFT and 1D 1H NOESY NMR allow the intermesogen ‘bend’ angles to be estimated. This has allowed the elucidation of a further structure property relationship, namely that the stability of the NTB phase exhibits a dependency on the bend angle of the molecule, satisfying an earlier theoretical treatment *[6]*.

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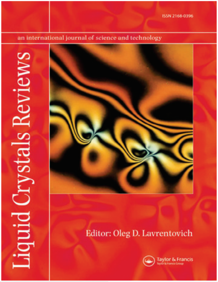

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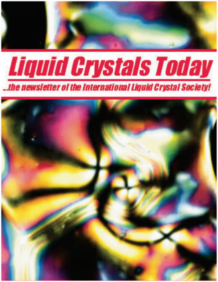

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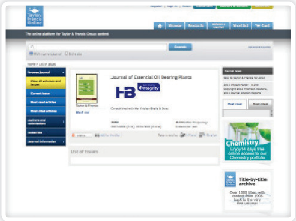

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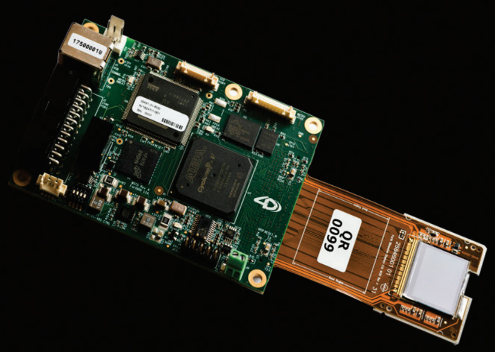

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