The British Liquid Crystal Society Conference 2014

BLCS 2014

Durham University

Monday 14th April to Wednesday 16th April 2014
Sponsors

BLCS and Durham University are very grateful to all our sponsors, who have helped make this conference possible.

Our major conference sponsors are Merck, who have supported the BLCS over many years.


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http://www.hull.ac.uk/kingston-chemicals/
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The first of two poster sessions this year is sponsored by OCF.

http://www.ocf.co.uk/
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OCF specialises in supporting the significant big data challenges of UK firms. Their in-house team and extensive partner network design, integrate, manage and host the high performance compute, storage hardware and analytics software necessary for customers to extract value from their data at low cost and without added complexity. With a 10-year heritage in HPC, OCF now works with over 20 per cent of the UK’s Universities, Higher Education Institutes and Research Councils, as well as commercial clients from a wide range of industries.
Sponsors

The second of our two poster sessions this year is sponsored by IBM.

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Key Information

Lectures
Will be in the Calman Learning Centre (CLC) on the University Science Site (see map of the University Science Site). The lecture theatre is the Rosemary Cramp Lecture Theatre on the 2nd floor of the CLC. Calman Learning Centre, University Science Site (Lower Mountjoy Site), Durham University, Durham, DH1 3HP.

Posters and the exhibition area
Will be in the Calman Learning Centre (CLC) on the University Science Site (see map of the University Science Site). The posters are on the top (4th) floor of the CLC in the Derman Christopherson Room and the Kingsley Barrett Room.

Registration
Will be in the Calman Learning Centre (CLC) on the University Science Site from 11.30 on Monday 14th April

Lunches and coffee
Will be in the poster area.

Accommodation and dinners
Will be in Collingwood College (see main map)
Collingwood College, South Road, Durham, DH1 3LT.

Arrival by car
We recommend that you arrive at Collingwood College and park at the college. You should let the college porters know your registration number to avoid clamping. If you arrive before 2 pm on Monday 14th April, we recommend that you leave your bags at the college (a room is reserved for this) and check in later. If you arrive after 2 pm, you may directly check-in to your room. Special check in arrangements have been made for overseas visitors arriving early.

Arrival by public transport
If you arrive at the university earlier than 11:30 on Monday 14th April we recommend you go to Collingwood College, leave your bags at the college (a room is reserved for this) and check in later. If you arrive at or after 11:30, it is probably best to bring your bags directly to the conference venue, the Calman Learning Centre (CLC) on the University Science Site; as lunch is available from 12:00. The Ken Wade lecture theatre has been reserved for you to leave your bags at the CLC. Special check in arrangements have been made for overseas visitors arriving early.

Arrival at the train station
Coming from the South you will arrive at platform 2. Exiting the station at platform 2 you can find taxis waiting immediately outside the station. Coming from the North you will arrive at platform 1. You should cross under the station to platform 2 to find a taxi. The taxi fare will be approximately £4. For those wanting to arrive via bus, the X1 service runs from the bus station (5 minutes walk from the train station) every 30 minutes, stopping at the University Science Site (Lower Mountjoy site).

Walking from the train station
On a nice day you may wish to walk from the train station either via town or via the river. (See main map for directions.) It is about a 35 minute walk to the University Science Site.
Talks
Invited talks are 40 minutes, plus 5 minutes for questions.
Contributed talks are 15 minutes, plus 5 minutes for questions.
The two closing talks are 25 minutes, plus 5 minutes for questions.

A computer will be provided with powerpoint (office 2010), libreoffice (version 4.2), acrobat reader (version 10). If you would like to use this facility then please upload your talk to the laptop before your session (please identify that you are a speaker at registration).

Alternatively, you may use your own laptop to present the talk.

Posters
Posters should include the following information at the top, in addition to your scientific content:
1. The title of your poster;
2. The names of all authors, but with the presenting author name made prominent,
3. The name and address of the institute(s) where you work.
The poster board dimensions are 1189mm (height) x 841mm (width). Posters must be attached only to your assigned poster board using velcro strips, which will be provided. Please put your poster up at the start of the conference during registration. Posters will remain up for the whole for the conference.

Poster presenters should present odd numbered posters in poster session 1, and even numbered posters in poster session 2.

Some Local Taxi Firms
Paddy's Taxis, Frankland Lane, Durham, County Durham, DH1 5TA  Tel: 0191 3866662
Mac’s Taxis, Sherburn Road, Durham, DH1 2JW  Tel: 0191 384 1329
Pratt’s Taxis, Maven House, Frankland Lane, Durham, DH1 5TA,  Tel: 0191 386 0700
Polly's Taxis, Tel: 07774 63 47 65
Bills Taxis, 24 Pilgrims Way, Durham, County Durham, DH1 1HB,  Tel: 0191 3867450
Map of the University Science Site

- Venue for BLCS committee meetings (Material's Chemistry Building Room MC106)
- South Road entry to Science Site
- up the hill to Collingwood College (10 mins walk)
- Conference lectures and posters held in the Calman Learning Centre
- To the town centre and the cathedral
- Stockton Road entry to Science Site

- South Road entry to Science Site
- MapBofBtheBUniversityBScienceBSite
- ConferencelecturesBandBpostersheldBintheBCalmanBLearningBCentre
- (Material'sChemistryBuildingRoomMC106)
Walking Distances

Elvet Riverside to Mountjoy - 10 mins. approx.

Hill Colleges to Market Place - 25 mins. approx.

Railway Station to Market Place - 15 mins. approx.
Welcome to Durham

Dear Delegate,

Welcome to Durham! I'm really pleased to welcome you to Durham for the annual British Liquid Crystal Society Conference (BLCS). This is the 28th BLCS conference: a sequence stretching all the way back to the 1980s. As usual we have a mix of science from across the liquid crystal community in the UK, and we are very pleased also to welcome distinguished colleagues from outside the British Isles to present their work.

The BLCS has always been a friendly society, where physicists, chemists, engineers and mathematicians have been able to work together, where academics and industrialists can meet, and where young scientists are welcomed and encouraged. Particularly, we value the opportunity for those presenting their own science for the first time (in talk or poster) to speak to some of the research leaders in the field about their work.

As usual we have a mix of longer invited talks and shorter talks, and we have a wide range of poster presentations. We very much hope you will enjoy the event, and you will come back and visit us in Durham in the future.

Yours sincerely,

Mark Wilson
Local Conference Organiser

About the conference

The conference will be held on the University Science Site, with accommodation provided in the nearby Collingwood College. The local organiser is Prof. Mark Wilson, Department of Chemistry, Durham University.

About Durham

Durham is England's third oldest university. It has been a place of learning since the 7th century: "The Father of English History", the Venerable Bede, wrote his "Historia ecclesiastica gentis Anglorum" in nearby Jarrow. Durham is a beautiful city with a UNESCO World Heritage Site at its heart centred around Durham Cathedral one of Europe's greatest medieval buildings.

'If you have never been to Durham before, go there at once. Take my car, it's wonderful.'

Bill Bryson’s Notes From a Small Island
Collingwood College

“Aime le Meilleur”, (Love the Best)

Collingwood College is a relatively modern college. It was founded in 1972 as the first mixed college in Durham University and named in memory of Sir Edward Collingwood. It is known as one of the friendliest colleges at the University. The academic community numbers around 1100 undergraduates and postgraduates, from all over the world - with more than 500 living in College. In addition to academic life, Collingwood students reveal a remarkable range of talents - in arts, sport, theatre, and helping others in the wider community - ensuring a constant buzz of activity.

Notable college alumni include James Cary (TV and radio writer), Benjamin Cook (journalist and author), Joe Crabtree (drummer of the band Wishbone Ash), Stephen Davies (children's author), Peter Elleray (Formula One and Le Mans race car designer), Mark Elliott (travel author), Jonah Fisher (BBC Journalist), Tim FitzHigham (British comedian), Lorraine Heggessey (controller of BBC One 2000-2005), Rt. Rev Nick Holtham (Bishop of Salisbury), Amjad Hussain (Rear Admiral, Royal Navy), Alex Loudon (Warwickshire and England cricketer), Sarah Keith-Lucas (BBC Weather presenter), David Kershaw (CEO of M&C Saatchi), Rt. Hon Lord Justice Andrew McFarlane (High Court Judge, Lord Justice of Appeal), Stephen Rowbotham (Olympic rower), Jonny Saunders (BBC Radio 2 sports presenter), Will Smith (Durham County Cricket Club cricketer), David Sproxton (joint founder of Aardman Animations) and Chris Terrill (Documentary maker, writer and adventurer).

A bit about the local organisers

This year the BLCS is being organised by the Durham Centre for Soft Matter (DCSM). The DCSM covers both experimental and theoretical soft matter research, which includes liquid crystals in addition to polymers, colloids, lyotropic systems, membranes and gels. The DCSM joint hosts (with Leeds and Edinburgh) the SOFI CDT (Centre for Doctoral Training), which offers at least 16 studentships a year to those interested in a PhD in soft matter and functional interface research; providing industrially-integrated, postgraduate training in research, enterprise and innovation for future leaders in the soft matter industrial sector.

Links

https://www.dur.ac.uk/soft.matter/
https://www.dur.ac.uk/soft.matter/cdt/
While you are in Durham...

If you have spare time on your visit, why not take a trip to see some of the local sites, that make this part of the UK so special. Durham itself is steeped in history. At the heart of Durham is the UNESCO World Heritage Centre encompassing the Cathedral, the Castle and Palace Green. Durham's cathedral dates back from the late 11th century. It was built in 1093 to house the Shrine of St Cuthbert, and so Durham Cathedral has been a place of pilgrimage, worship, welcome and hospitality for almost a millennium. The city itself has many places to visit, and many places to enjoy beautiful walks.

For those with a car and a little more time, the North East of England offers some of the most stunning countryside in the UK, which is steeped in history. We are not far from Hadrian's wall (1 ¼ hour drive), from the beautiful Northumberland coast - including Holy Island (1 ¼ hour drive) and Bamburgh Castle, nature reserves such as Hawthorn Dean on the coast (30 mins drive) and Witton-le-Wear in land (30 mins drive), and High Force Waterfall (50 min drive). The world famous Beamish Museum (20 mins drive), telling the story of the people of the North East, is a short drive away.

Some Durham sites...

**Durham Cathedral** (20-25 minutes walk down hill from Collingwood College)

The Cathedral is open to the public to 6.00pm Monday to Saturday; and 5.30pm on Sunday. You may want to visit:

- The Cathedral Church
- The Tower
- The Cloister
- The Monks' Dormitory
- The West Undercroft
- The Chapel of the Holy Cross

**Durham Castle** (20-25 minutes walk down hill from Collingwood College)

Construction of the Castle began in 1072 under the orders of William the Conqueror, six years after the Norman Conquest of England, and soon after the Normans first came to the North. The construction took place under the supervision of the Earl of Northumberland, Waltheof, until he rebelled against William and was executed in 1076. The castle then came under the control of the Bishop of Durham, Walcher, who purchased the earldom and thus became the first of the Prince-Bishops of Durham, a title that was to remain until the 19th century, and was to give Durham a unique status in England. The Castle is home to University College, the oldest of Durham University's colleges (founded in 1837).

Outside of University Terms, tours are normally available most mornings of the week at 10:00, 11.00 and 12:00, and in the afternoons when there are no commercial activities, from 14:00 to 17:00. Please contact the Palace Green Library on: +44 (0)191 334 2932 to check information on the current times and dates of tours.
The Riverside Walks (20 minutes walk downhill from Collingwood College)
The Riverside Walks offer stunning views of the Cathedral and the City.

The Botanical Gardens (less than 5 minutes walk from Collingwood College)
Our 10 hectare university botanic garden is set amongst beautiful mature woodlands near Collingwood College. It houses plant collections from around the world, including China, Japan, North America, South Africa, New Zealand and Chile, as well as a woodland garden, alpine garden and bamboo grove. Don't miss the magnificent monkey puzzle tree that dominates the centre of the garden. In the glasshouses you will find a collection of tropical rainforest plants (including the giant Amazonian water lily, *Victoria amazonica*), desert plants, and more familiar plants from the Mediterranean.

Opening times:
- 10am to 4pm (November until the end of February)
- 10am to 5pm (March until the end of October)

The Oriental Museum (less than 5 minutes walk from Collingwood College)
The Oriental Museum is the only museum in the North of Britain devoted entirely to the art and archaeology of the Orient. The Chinese and Egyptian collections are among the finest to be found anywhere in Britain.

Opening times:
- Monday – Friday 10am to 5pm
- Saturday – Sunday 12 pm to 5 pm
- Bank Holidays 12 pm to 5 pm

Durham Museum & Heritage Centre (20 minutes walk downhill from Collingwood College)
The Museum tells the story of the City of Durham from medieval times to the present day. The museum is situated in an historic church next to the World Heritage Site of Durham Cathedral and Castle.

Opening times:
- April – May W/ends & Bank Holidays 2 pm to 4:30pm
- June – Sept Daily 11am to 4.30pm
Programme for BLCS 2014
Monday 14th April 2014

11:30 to 13:00 Registration Desk in the foyer of Calman Learning Centre (CLC), University Science Site.
(For those coming by car, car parking will be provided at Collingwood College. You may leave your car and luggage at Collingwood College, please make sure to check in your luggage and register your car at the porter's lodge in the entrance to the college. For those travelling by train and wanting to arrive directly at the University Science Site, a room will be provided (Ken Wade lecture theatre) to store your luggage for the afternoon before transferring to Collingwood College for dinner.)

12:00 to 13:05 Lunch in Derman Christopherson,
(For Committee Members only)
lunch and poster setup (Derman Christopherson and Kingsley Barrett rooms)
-posters will remain up for viewing throughout the conference, please make sure to put your poster up during conference registration,
-tea and coffee will be available with lunch.

11:45 – 13:00 BLCS Committee Meeting (for Committee Members only) in room MC106 in the Materials Chemistry Building (directly opposite the CLC). Lunch will be available for the committee in MC106.

Rosemary Cramp Lecture Theatre (CLC) – session 1: 13:10 to 17:00

<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
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</thead>
<tbody>
<tr>
<td>13:10-13:15</td>
<td>Opening and Welcome</td>
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<tr>
<td>13:15-14:00</td>
<td>Plenary 1: Randall D. Kamien (University of Pennsylvania)</td>
</tr>
<tr>
<td>14:00-14:20</td>
<td>Talk 1: Timothy J. Atherton (Tufts University)</td>
</tr>
<tr>
<td>14:20-14:40</td>
<td>Talk 2: Doug Cleaver (Sheffield Hallam University)</td>
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<tr>
<td>14:40-15:05</td>
<td>Coffee/Tea/Scones in Christopherson/Barrett Rooms (CLC)</td>
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<tr>
<td>15:05-15:50</td>
<td>Plenary 2: Dave Walba (University of Colorado)</td>
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<tr>
<td>15:50-16:10</td>
<td>Talk 3: Ingo Dierking (University of Manchester)</td>
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<tr>
<td>16:10-16:30</td>
<td>Talk 4: Nicholas Kasch (University of Manchester)</td>
</tr>
<tr>
<td>16:30-16:50</td>
<td>Talk 5: Rachel M. Hyman (University of Cambridge)</td>
</tr>
<tr>
<td>16:50-17:00</td>
<td>AGM</td>
</tr>
</tbody>
</table>

Derman Christopherson / Kingsley Barrett – poster session 1 - 17:00 to 18:30
-refreshments, cold drinks, wine and nibbles available
$poster presenters should stand by odd numbered posters in this session$

Transfer to Collingwood College
18:30 onwards, pick up keys in Collingwood
18:30-19:15 bar available in Collingwood
19:15-20:15 Dinner in the dining room at Collingwood
20:15 onwards – bar in Collingwood until standard closing time.
### Tuesday 15th April 2014

#### 7:30 to 8:45 Breakfast – Collingwood
Transfer to Calman Learning Centre

**Rosemary Cramp Lecture Theatre (CLC) – session 2: 9:00 to 12:40**

<table>
<thead>
<tr>
<th>Time</th>
<th>Event Description</th>
<th>Speaker/Institution</th>
<th>Topic</th>
</tr>
</thead>
<tbody>
<tr>
<td>9:00 – 9:45</td>
<td>Plenary 3</td>
<td>Andrew Masters (University of Manchester)</td>
<td>Molecular theories of liquid crystals: -some applications and speculations</td>
</tr>
<tr>
<td>9:45 – 10:05</td>
<td>Talk 6</td>
<td>Vasily Oganesyan (University of East Anglia)</td>
<td>Probing nematic and discotic liquid crystals by a combination of EPR spectroscopy and theoretical modelling</td>
</tr>
<tr>
<td>10:05 – 10:25</td>
<td>Talk 7</td>
<td>Chloe Tartan (University of Oxford)</td>
<td>Hybrid Aligned Nematic Based Measurement of Flexoelectric Coefficient $e_1 + e_3$</td>
</tr>
<tr>
<td>10:25 – 10:50</td>
<td>Coffee/Tea/Scones in Christopherson/Barrett Rooms (CLC)</td>
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</tr>
<tr>
<td>10:50 – 11:35</td>
<td>Plenary 4</td>
<td>Igor Muševič (University of Ljubljana)</td>
<td>Light-Driven Creation of Topological Monopoles in a Nematic Liquid Crystal</td>
</tr>
<tr>
<td>11:35 – 12:20</td>
<td>Plenary 5</td>
<td>BLCS Young Scientist Award Lecture – Gareth Alexander (University of Warwick)</td>
<td>Applied Topology: Textures in Liquid Crystals</td>
</tr>
<tr>
<td>12:20 – 12:40</td>
<td>Talk 8</td>
<td>Flynn Castles (University of Oxford)</td>
<td>Reaction-diffusion in liquid crystals</td>
</tr>
</tbody>
</table>

#### 12:40 to 13:40 Lunch in Derman Christopherson.
- lunch and posters (Derman Christopherson and Kingsley Barrett rooms)
- tea and coffee available for lunch

#### 12:40 – 13:40 BLCS Committee Meeting (for Committee Members only) in room MC106 in the Materials Chemistry Building (directly opposite the CLC). Lunch will be available for the committee in MC106.
<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
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</thead>
<tbody>
<tr>
<td>13:40 – 14:00</td>
<td>Talk 9&lt;br&gt;Simon M. Wood (University of Oxford)&lt;br&gt;Adaptive holographic pumping of liquid crystal lasers</td>
</tr>
<tr>
<td>14:00 – 14:20</td>
<td>Talk 10&lt;br&gt;Harry E. Milton (University of Manchester)&lt;br&gt;Liquid crystal contact lenses to correct presbyopia</td>
</tr>
<tr>
<td>14:20 – 14:40</td>
<td>Talk 11&lt;br&gt;Malik M. Qasim (University of Cambridge)&lt;br&gt;Polariser free optically activated shutter</td>
</tr>
<tr>
<td>14:40 – 15:00</td>
<td>Talk 12&lt;br&gt;Tom P. Bennett (University of Southampton)&lt;br&gt;Multiscale models of liquid crystals dispersions of nanoparticles</td>
</tr>
<tr>
<td>15:00 – 15:25</td>
<td>Coffee/Tea/Scones in Christopherson/Barrett Rooms (CLC)</td>
</tr>
<tr>
<td>15:25 – 16:10</td>
<td>Plenary 6&lt;br&gt;The 2014 Sturgeon Lecture&lt;br&gt;Oleg D. Lavrentovich (Kent State)&lt;br&gt;Lyotropic chromonic liquid crystals: From viscoelasticity to topological turbulence</td>
</tr>
<tr>
<td>16:10 – 16:30</td>
<td>Talk 13&lt;br&gt;Armando Navarro-Vázquez&lt;br&gt;(Universidade de Vigo)&lt;br&gt;Cromolyn. A suitable weak NMR weak-aligning medium for small molecules</td>
</tr>
<tr>
<td>16:30 – 16:50</td>
<td>Talk 14&lt;br&gt;Chris Welch (University of Hull)&lt;br&gt;New materials exhibiting non-ionic lyotropic chromonic mesophases</td>
</tr>
<tr>
<td>16:50 – 17:10</td>
<td>Talk 15&lt;br&gt;Anna Akinshina (University of Manchester)&lt;br&gt;Challenges in atomistic modelling of chromonic TP6EO2M molecules</td>
</tr>
</tbody>
</table>

**Derman Christopherson / Kingsley Barrett – poster session 2 - 17:10 to 18:30**
- refreshments, cold drinks, wine and nibbles
   (poster presenters should stand by even numbered posters in this session)

**Transfer to Collingwood**
18:30-19:15 bar
19:15-21:30 Conference Banquet in Collingwood College
21:30-onwards – bar in Collingwood until 00:00
Wednesday 16th April 2014

7:30 to 8:45 Breakfast – Collingwood
A room is available in Collingwood for luggage for those leaving from Collingwood College.

Transfer to Calman Learning Centre
The Ken Wade lecture theatre is available for leaving luggage for those leaving from Calman learning centre.

Rosemary Cramp Lecture Theatre (CLC) – session 4: 9:00 to 12:40

<table>
<thead>
<tr>
<th>Time</th>
<th>Talk</th>
<th>Presenter</th>
<th>Title</th>
</tr>
</thead>
<tbody>
<tr>
<td>9:00 – 9:20</td>
<td>Talk 16</td>
<td>Faleh Z. Al-Qahtani (University of Hull)</td>
<td>Synthesis and investigation of rod-shaped mesogens functionalized with ethylenoxy chains and attachment to gold nanoparticles</td>
</tr>
<tr>
<td>9:20 – 9:40</td>
<td>Talk 17</td>
<td>David Allen (University of Hull)</td>
<td>Synthesis and properties of dimeric materials with lateral and terminal fluorine substituents for dual frequency liquid crystal mixtures</td>
</tr>
<tr>
<td>9:40 – 10:00</td>
<td>Talk 18</td>
<td>Z. Ahmed (University of Hull)</td>
<td>The investigation of dimeric materials with a nematic – nematic phase transition</td>
</tr>
<tr>
<td>10:00 – 10:20</td>
<td>Talk 19</td>
<td>James Hussey (University of Hull)</td>
<td>The investigation of novel photochromic liquid crystals based on the 2,4,5-triphenyl imidazole dimer group</td>
</tr>
<tr>
<td>10:20 – 10:45</td>
<td></td>
<td>Coffee/Tea/Scones in Christopherson/Barrett Rooms (CLC)</td>
<td></td>
</tr>
<tr>
<td>10:45 – 11:30</td>
<td>Plenary 7</td>
<td>John Goodby (University of York)</td>
<td>What makes a liquid crystal?</td>
</tr>
<tr>
<td>11:30 – 12:00</td>
<td>Talk 20</td>
<td>Timothy D. Wilkinson (University of Cambridge)</td>
<td>Graphene electrodes for liquid crystal devices in the mid-infrared</td>
</tr>
<tr>
<td>12:00 – 12:30</td>
<td>Talk 21</td>
<td>John Lydon (University of Leeds)</td>
<td>Cordite, cine film and exploding billiard balls: cellulose esters and their mesogenic properties</td>
</tr>
<tr>
<td>12:30 – 12:40</td>
<td></td>
<td>Closing and Prizes</td>
<td></td>
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</tbody>
</table>

12:40 to 13:40 Lunch in Derman Christopherson,
-tea and coffee available for lunch

Conference End
<table>
<thead>
<tr>
<th>BLCS 2014 talks</th>
<th>presenting author</th>
<th>other authors</th>
<th>affiliations</th>
</tr>
</thead>
<tbody>
<tr>
<td>I2 Structure of the helical nanofilament phase, and possible applications in organic electronics</td>
<td>David M. Walba</td>
<td></td>
<td>Department of Chemistry and Biochemistry and the Liquid Crystal Materials Research Center, 215 UCB, University of Colorado, Boulder, Colorado 80309-0215, USA</td>
</tr>
<tr>
<td>I3 Molecular theories of liquid crystals – some applications and speculations</td>
<td>A J Masters</td>
<td>M.Nikkhou, M.Škarabot, S.Čopar, M.Ravnik, S.Žumer</td>
<td>School of Chemical Engineering &amp; Analytical Science, University of Manchester, Manchester, M13 9PL, UK</td>
</tr>
<tr>
<td>I4 Light-Driven Creation of Topological Monopoles in a Nematic Liquid Crystal</td>
<td>Igor Muševič</td>
<td></td>
<td>Condensed Matter Physics Department, Jožef Stefan Institute, Jamova 39, 1000 Ljubljana, Slovenia</td>
</tr>
<tr>
<td>I5 Applied Topology: Textures in Liquid Crystals</td>
<td>Gareth P. Alexander</td>
<td></td>
<td>Department Physics and Centre for Complexity Science, University of Warwick, Coventry, CV4 7AL, UK</td>
</tr>
<tr>
<td>I6 Lyotropic chromonic liquid crystals: From viscoelasticity to topological turbulence</td>
<td>Oleg D. Lavrentovich</td>
<td></td>
<td>Liquid Crystal Institute, Kent State University, Kent, Ohio 44242, USA</td>
</tr>
<tr>
<td>I7 What Makes a Liquid Crystal?</td>
<td>John W. Goodby</td>
<td></td>
<td>Department of Chemistry, University of York, York YO10 5DD, UK</td>
</tr>
<tr>
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<tr>
<td>T1 Simulating defect textures on relaxing nematic shells</td>
<td>Timothy J. Atherton</td>
<td>B.Mbanga, K.Voorhes</td>
<td>Department of Physics and Astronomy, Tufts University, 5 Colby Street, Medford, Massachusetts, USA 02155</td>
</tr>
<tr>
<td>T2 Towards independent control of polar and azimuthal anchoring</td>
<td>Doug Cleaver</td>
<td>C.Anquetil-Deck, J.Bramble, T.Atherton</td>
<td>Institute of Physical Chemistry, University of Stuttgart, Pfaffenwaldring 55, 70569 Stuttgart, Germany; Department of Chemistry and Biochemistry, University of Colorado, Boulder, CO80309, USA; School of Physics and Astronomy, University of Manchester, Oxford Road, Manchester M139PL, UK</td>
</tr>
<tr>
<td>T3 Alyotropic chiral SmC liquid crystal with polar switching</td>
<td>Ingo Dierking</td>
<td></td>
<td>School of Physics and Astronomy, The University of Manchester, Manchester, M13 9PL, UK; School of Chemistry, University of Manchester, Oxford Road, Manchester</td>
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<td>I. Dierking, M.Turner</td>
<td>Department of Engineering, University of Cambridge, Cambridge, CB3 0FA, UK; Technical University of Berlin, Department of Chemistry, Str. Des 17. Juni 124, 10623 Berlin, Germany; Department of Engineering Science, University of Oxford, Oxford, OX1 3PJ</td>
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<td>A.Lorenz, S.M.Morris, T.D.Wilkinson</td>
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<td>F.Chami, H.Gopee, A.N.Cambridge, M.R.Wilson</td>
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<td>S.J.Elston</td>
<td>Department of Engineering Science, University of Oxford, Parks Road, Oxford, OX1 3PJ</td>
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<td>P.B.Morgan, J.H.Clamp, H.F.Gleeson</td>
<td>School of Physics and Astronomy, University of Manchester, Manchester, M13 9PL, UK; Eurolens Research, University of Manchester, Manchester, M13 9PL; UltraVision CLPL, Leighton Buzzard, LU7 4RW</td>
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<td>School of Chemical Engineering &amp; Analytical Science, The University of Manchester, Oxford Road, Manchester, M13 9PL; Department of Chemistry, Durham University Science Laboratories, South Road, Durham DH1 3LE</td>
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<td>Department of Materials Science and Engineering, University of Sheffield, Sheffield, S1 3JD, UK; Institute of Organic Chemistry, Martin-Luther University, Halle, Germany</td>
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<td>Department of Materials Science and Engineering, University of Sheffield, Sheffield S1 3JD. Institute of Multidisciplinary Research for Advanced Material, Tohoku University, Sendai 980-8577, Japan</td>
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I will discuss the homotopic classification of topological defects in liquid crystals with special attention to systems with broken translational symmetry. In the simplest case of smectics, we can see that this classification breaks down and needs repair or reformulation. I will discuss the latter and show how it leads to a surprising, underlying symmetry in smectic ground states. In related work epitaxially assembled toric focal conic domain (TFCD) arrays of smectic-A liquid crystals onto pillar arrays. The 3D nature of the pillar array is crucial to confine and direct the formation of TFCDs on the top of each pillar and between neighboring pillars, leading to highly ordered square and hexagonal array TFCDs persisting deeply into the bulk. Finally, exploiting our two experiences with these materials, we study the flower-like pattern shown on the left and develop new rules for tying together equally-spaced layers in thin films.

References
Structure of the helical nanofilament phase, and possible applications in organic electronics

David M. Walba, Noel A. Clark, Garry Rumbles, Rebecca Callahan, Ethan Tsai, Jacqueline M. Richardson, Michael T. Springer, Michi Nakata, Dong Chen and David Coffey

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Since its beginnings in the 19\textsuperscript{th} century chirality has played a central role in liquid crystal science. More recently, it has been shown that chirality drives the formation of the helical nanofilament (HNF) phase (a.k.a. B4 phase) - a novel organic nanoparticle system.\textsuperscript{1} The structure of this phase, composed of bent-core molecules, is illustrated below for the prototypical HNF mesogen NOBOW (P-9-O-PIMB). In the HNF phase, molecules form a unique hierarchical assembly of stacked layers (layer spacing ~ 50Å), possessing spontaneous negative Gaussian curvature.

![Layer face Layer edges]

Due to this curvature, the layers are self-limited in width (~ 30nm), and the stacks self-limited in layer number (~ 5-8), leading to nearly cylindrical HNFs ~ 30 nm in diameter, with no constraints on their length. Based upon solid state NMR data showing slow conformational dynamics over the entire temperature range of the phase (up to 155°C),\textsuperscript{2} it appears that individual layers are effectively single crystal, though there is no correlation of molecular positions across layers.

Exploration of the mesogen structure space providing the HNF phase, the fascinating stereochemistry of the system, results of solid state NMR experiments aimed at developing an improved understanding of the nature of the supramolecular structure in individual layers, and experiments speaking to the potential for application of these nanoparticles in solar energy conversion, will be described.

References


Molecular theories of liquid crystals – some applications and speculations

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Statistical mechanics seeks to predict the properties of bulk matter in terms of the properties of the constituent particles. In this talk, I would like to give a rather biased review on how far statistical mechanical theory, as opposed to computer simulation, has achieved this aim in the field of liquid crystals and then go on to give some rather wild speculations about what one might achieve in the future.

The theory of isotropic fluids is well-advanced. One can make quantitatively reliable predictions about the properties of complex mixtures. These advances have been based on the use of the virial expansion, integral equation theory and perturbation approaches around the well-characterised hard sphere fluid. There is naturally a lot of work yet to be done, but the field is in good shape.

The situation for even the simplest liquid crystalline phase, the nematic, is, however, not so well under control. The basis for much current research is Onsager’s second virial approach, approximately resummed using the methods of Parsons and Lee. The focus tends to be on symmetric, hard bodies (spherocylinders, platelets, etc.) and, as such, the primary applications are to colloidal systems. Higher order virials have also been calculated for such systems, which obviate the need for approximate scaling methods. I will give examples of recent uses of such methods in the calculation of the phase behaviour and elastic properties of various hard particle systems, including some calculation on the biaxial nematic phase.

It is still far from clear to what extent traditional integral equation theory, such as the Percus-Yevick and Hypernetted Chain equations, can be applied to liquid crystals. I will provide a brief analysis of the structure of the nematic bridge function and discuss why it is so hard to find a theoretically well-founded set of integral equations for ordered phases.

The above discussion focuses on the behaviour of simple particle models. While one may learn a lot of useful, fundamental science from these studies, it would also be nice to be able to make reliable predictions about complex, molecular systems. SAFT and modern versions of RISM integral equations have proved remarkably fruitful in dealing with the isotropic behaviour of molecular fluids. The talk will finish with speculations, and maybe even some preliminary results, as to whether such methods could make similar headway for thermotropic liquid crystals.

References
Light-Driven Creation of Topological Monopoles in a Nematic Liquid Crystal

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The electric charge of an elementary particle is a common example of a topological monopole that is the source of an electric field and causes the force between charged objects. In liquid crystals, a topological monopole is a singularity, or a defect, of a material field, which describes the orientation order of liquid-crystal molecules. Monopoles are abundant in nematic colloids, where they generate structural forces between the colloidal particles\textsuperscript{1,2}. Simple objects, like spheres or fibres with a perpendicular surface alignment of liquid-crystal molecules, usually carry a single defect in the form of a point or a ring with a unit topological charge. Complex objects, such as handlebodies, generate a larger number of topological defects that carry a precisely defined charge\textsuperscript{3}. We show that topologically simple objects, like a fibre (rod), can carry an arbitrary number of charge-neutral defect pairs\textsuperscript{4}. They are produced via the Kibble-Zurek mechanism of defect production after applying a laser-induced temperature quench. The pairs are long-lived, oppositely charged rings or points that can be precisely manipulated with laser tweezers. Two oppositely charged monopoles either attract and annihilate, or form a long-lived, charge-neutral loop made of two segments with a fractional topological charge. Our findings will help with the tailoring of new, topological, colloidal structures and demonstrate that the Kibble-Zurek mechanism is sensitive to the topology of the space that is occupied by the symmetry-breaking field.

References

Applied Topology: Textures in Liquid Crystals

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Liquid crystals have always been identified, understood and characterised by their rich and beautiful textures. In recent years, work on colloidal systems and advances in microfabrication have led to a considerable increase in the complexity of the textures that can be created and controlled. Their exploration and understanding is a form of applied topology, with great potential for the development of novel soft materials. I will summarise the work in this area, from blue phases to knots.
Lyotropic chromonic liquid crystals: From viscoelasticity to topological turbulence

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Lyotropic chromonic liquid crystal ((LC)$_2$ or simply chromonics) represent dispersions of organic molecules in water that self-organize into orientationally ordered phases thanks to non-covalent reversible aggregation [1]. Since the aggregates are bound by weak van der Waals forces, their length varies strongly with concentration, temperature, ionic content. The (LC)$_2$ are thus very different from a standard thermotropic LC with molecules of covalently fixed shape and from a lyotropic LC formed by polymers of fixed molecular weight. The presentation discusses (1) concentration and temperature behavior of viscoelastic properties of chromonics [2]; (2) symmetry breaking effects during phase transitions (chiral tactoids and proliferation of topological defects) [3] and (3) chromonics as the basis of living liquid crystals [4]. The studies of living liquid crystals reveal a wealth of new intriguing dynamic out-of-equilibrium phenomena, caused by the coupling between the bacteria activity-triggered flow and long-range orientational order of the medium. Among these are: (a) non-linear trajectory of the bacteria controlled by distorted director fields; (b) local melting of (LC)$_2$ by the rotating flagella; (c) birefringence enabled visualization of the motion of nanometer thick flagella; (d) activity-induced transition from an equilibrium state of a uniaxially aligned nematic to low-Reynolds-number turbulence through a periodically distorted nematic with a macroscopic length scale that depends on the elastic moduli and activity. The work is supported by NSF grants DMR 1104850 and 1121288.

Figure. (A,B) Equilibrium unidirectional state of a chromonic with inactive (immobilized) bacteria; (C,D) periodic undulations of the director cause by low-level activity of swimming bacteria; (E) increase of oxygen supply causes a transition from periodic undulations to topological turbulence with nucleating disclination pairs.

References
What Makes a Liquid Crystal?

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One of George Gray’s favourite songs was the liquid crystal anthem. It goes something like this:

Dear friends let’s ask what are these liquid crystals?
Mythical beasts with heads and tails, not blood or gristle
In flocks they fly with lashing tails and flashing eyes
In heat of day they fade away as they dye

What a mystery we see, Smectic A, Smectic B
What’s the pattern what’s the key
Smectic H, Smectic C
How diverse the combinations of distortions, of rotations be
No it is not clear at all to me

George was also clear about what he considered to be a liquid crystal and what was not. The last verse of the song implies at the time we did not understand the smectic state, however, this was beautifully resolved through defined geometric or exponential decay in order that occurred in the melting process. This understanding produced a complete classification and unification of the smectic state.

Since then similar developments have occurred with respect to chirality in smectics and nematics\(^1\). Thus, for phases composed of relatively small rod-like molecules unification of the nomenclature system has been a great success, one that was attempted or assumed to be reproducible for systems composed of molecules that have more complicated structures. For example, H-bonding materials found in glycolipids\(^2\), super- and supra-molecular materials\(^3\), and nano-particulate liquid crystals\(^4\) to name but a few. In order to understand organization and structure in such systems it is first necessary to understand the effects of molecular complexity\(^5\), micro- and nano-segregation\(^6\), and the amplification and transmission of properties\(^7\).

However, two issues have complicated our understanding of larger molecular systems or materials composed of molecules of unusual molecular shape as follows; (i) the compounding of physical properties with structure, and (ii) the effect of the slowing of dynamic molecular motions on thermodynamic versus kinetic processes. Moreover, changing length scales can have pronounced effects on the very nature of liquid crystallinity, such that periodicity for liquid crystals is no longer necessary to be related to molecular structure. This presentation will attempt to develop a more complete understanding of liquid crystals over all length scales.

References
Simulating defect textures on relaxing nematic shells

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Two nematic shells brought in contact coalesce in order to reduce their interfacial tension. This process proceeds through the creation of a liquid neck-like bridge through which the encapsulated fluid flows. Following this topological transition, we study the defect textures as the combined shell shape relaxes. Varying the sizes of the shells, we perform a quasistatic investigation of the director field and the defect valence on the doublet. Regimes are found where positive and negative defects exist due to the large negative Gaussian curvature at the neck. Using large-scale computer simulations, we determine how annihilating defect pairs on coalescing shells are selected, and the stage of coalescence at which annihilation occurs.
Towards independent control of polar and azimuthal anchoring\textsuperscript{1}

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Monte Carlo simulation, experiment, and continuum theory are used to examine the anchoring exhibited by a nematic liquid crystal at a patterned substrate comprising a periodic array of rectangles that, respectively, promote vertical and planar alignment. It is shown that the easy axis and effective anchoring energy promoted by such surfaces can be readily controlled by adjusting the design of the pattern. The calculations reveal rich behaviour: for strong anchoring, as exhibited by the simulated system, for rectangle ratios $\geq 2$, the nematic aligns in the direction of the long edge of the rectangles, the azimuthal anchoring coefficient changing with pattern shape. In weak anchoring scenarios, however, including our experimental systems, preferential anchoring is degenerate between the two rectangle diagonals. Bistability between diagonally aligned and edge-aligned arrangement is predicted for intermediate combinations of anchoring coefficient and system length scale.

Reference
A lyotropic chiral SmC liquid crystal with polar switching[1]

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While thermotropic and lyotropic liquid crystal systems are often treated separately, there are quite often strong similarities concerning their phase structure and symmetry, as for example in the case of the SmA and the lamellar L\textsubscript{α} phase. It is thus surprising that reports about the tilted SmC analogue have hardly ever been published for lyotropic liquid crystals (fig.1), and certainly no analogue of the chiral tilted SmC phase, which in the world of thermotropic liquid crystals is commonly known as a ferroelectric liquid crystal (FLC), due to the occurrence of a spontaneous polarization and polar electrooptic switching.

We demonstrate a lyotropic ferroelectric liquid crystal from a chiral diol with a phenylpyrimidine core. The phase diagram with water is determined, and a variety of experimental techniques are used to demonstrate the tilted nature of the phase. These are in particular texture observations of Schlieren textures, which show s=+1 and s=−1 defects exclusively. Also the typical ferroelectric texture of zigzag defects is observed, as is the domain texture which results from molecular tilt in opposite directions. A second employed experimental technique is 2D x-ray diffraction and measurements of the d-spacing. The observed behaviour is characteristic of a standard SmC to SmA phase transition with a decreasing tilt angle for increasing temperature at a constant solvent concentration.

Macroscopic chirality is shown from the equidistance line pattern which results from the compensation of the spontaneous polarisation. The pitch of the helical superstructure lies in the order of a few micrometres, increasing as the transition to the SmA phase is approached. Chiral information, i.e. the helical twist of the tilt direction is thus surprisingly communicated across the mediating layer of achiral water. At last, while we were not able to directly measure a spontaneous polarization, due to the high ionic conductivity, we demonstrate polar electrooptic switching as it is normally observed for the FLC phase of thermotropic liquid crystals. The electrooptic modulation is sensitive to the sign of the applied electric field, and the modulation depth resembles that of the temperature dependence of the tilt angle.

In conclusion, we have demonstrated the remarkable observation of a tilted lyotropic phase with macroscopic chirality and polar electrooptic switching, thus, the first observation of a lyotropic surface stabilized ferroelectric liquid crystal. This observation is the more remarkable, as the chirality information needs to be communicated across intermediate layers of water or other achiral solvents.

The liquid crystalline blue phase stabilised by non-mesogenic and fluorescent oligomers

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The 'blue phases', which can be formed by chiral molecules at temperatures between those of the chiral nematic and isotropic phases,\textsuperscript{1} are potentially useful materials\textsuperscript{2} with the drawback that they are normally only stable in a temperature range of less than 1K. A number of methods have been found to stabilise the blue phase over a larger temperature range, notably the polymerisation of monomer molecules inside a blue phase liquid crystal.\textsuperscript{3} We have demonstrated an increase in the blue phase stability range from 0.5K to 12K by simply mixing a liquid crystalline compound with polystyrene of low molecular weight.\textsuperscript{4} These results are distinctive in that they are measured on heating, eliminating any supercooling effects, and that the dependence of the stability range on concentration and molecular weight is captured well by a simple theoretical model. In addition we have demonstrated effective stabilisation in a range of up to 7K using a fluorescent oligomer. Since the proposed cause of the stabilisation is microscopic phase separation on the photonic length scale, fluorescence could provide a way of probing this structure. One could imagine mixed systems such as this enhancing the photonic properties of the blue phase.

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Polymer stabilised blue phase liquid crystals are known to be fast switching, optically isotropic materials but their ability to phase modulate light had not been investigated until recently. A high speed continuous phase modulating material is important for high quality spatial light modulating (SLM) devices. Such devices are used in computer-generated holograms, optical correlators, optical tweezing and many other applications.\[1\] Continuous phase modulation is preferred to intensity modulation for most of these applications as it is a more efficient and allows the removal of the zero order and the 180° conjugate image otherwise present.\[2,3\] For full correction in adaptive optics applications, modulation of greater than one wavelength is required. High speed is desired for the use in high frame rate applications.

Liquid crystal on silicon (LCoS) SLM devices offer easier and cheaper manufacturing compared to the micro-mirror counterparts. However, the devices are limited by the properties of the liquid crystal being used. Currently, a material with both fast switching and continuous phase modulation is not available. Nematics offer the continuous phase modulation but are slow switching (10-100ms). Ferroelectrics are capable of high speed switching (10-100μs) but only offer binary phase modulation.\[1,3\]

Initial experimental work carried out by the authors on the properties of the blue phase, demonstrated that it can continuously phase modulate light at high speed and is insensitive to the angle of incident light polarisation, figure 1. This paper builds on the original findings, to also consider full polarisation characterisation, including circular polarisation. The material is optically isotropic at the wavelength being used and so it is hoped that the response will be independent of incident polarisation state. The effect of the response due to different platelet orientations will be investigated by looking at the effect of different sizes of platelets. We will also investigate the temperature dependency.

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{figure1.png}
\caption{Phase modulation of light by a blue phase liquid crystal at different angles of input light polarisation}
\end{figure}

References:
Probing nematic and discotic liquid crystals by a combination of
EPR spectroscopy and theoretical modelling
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Electron Paramagnetic Resonance (EPR) with paramagnetic spin probes (SP) is a particularly valuable advanced spectroscopic method for studying both structure and dynamics of soft matter systems such as liquid crystals (LC) [1].

In this presentation we report our recent application of variable temperature EPR spectroscopy combined with theoretical modelling to both nematic and discotic LCs. Such an approach bridges the gap between theory and experiment allowing unambiguous interpretation of EPR lineshapes and enabling conclusions to be drawn about molecular motions and order in the bulk phase [2,3].

For nematic LCs structurally variable nitroxide SPs probing different aspects of LC dynamics have been employed resulting in different but highly complementary EPR spectra. For a range of temperatures EPR spectra of LCs doped with SPs are predicted directly from fully atomistic Molecular Dynamics (MD) simulations using our novel MD-EPR simulation methodology [2]. They show excellent agreement with experiment. Using MD-EPR approach we were able to characterise in detail the dynamics and molecular organisation in different phases of nematic LCs [3,4]. In particular, we were able to predict and confirm experimentally dynamic fluctuations between partially ordered and disordered meta-stable states at the phase transition critical points [3,4].

We also present the first application of EPR spectroscopy to columnar discotic liquid crystal (HAT6) using a novel rigid-core nitroxide spin probe designed and synthesized by us for this purpose (see picture below) [5]. EPR spectra measured at different temperatures across three phases show a strong sensitivity to the HAT6 phase composition, molecular rotational dynamics, and columnar order as well as the director distribution. Simulation of the EPR line shapes using a Brownian Dynamics (BD) simulation model gives a numerical estimate of these parameters at different temperatures along both I-Col and Col-Cr phase transitions.

References
Hybrid Aligned Nematic Based Measurement of Flexoelectric Coefficient 

$e_1 + e_3$

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In the flexoelectric effect, a net electric polarization is induced by a mechanical deformation of the director field that defines the molecular orientation in a liquid crystal material. A hybrid aligned nematic (HAN) liquid crystal cell is characterized by homeotropic molecular alignment at one boundary surface and homogeneous planar alignment at the other. The distortion field of such a device is potentially useful for the measurement of flexoelectric polarization$^1$.

Applying positive and negative DC fields reveal sign-dependent responses attributed to flexoelectricity and sign-independent responses that are largely dielectric. Under AC fields, first and second harmonics are related to the flexoelectric and dielectric effects respectively. In a strong anchoring limit, the flexoelectric polarization gives rise to an effective voltage shift or offset, inducing asymmetry between positive and negative voltages$^2$. However, on account of different surface alignment polarities, difficulties arise in the separation of different polar terms. Additionally, ions present in the liquid crystal lead to screening of the electric field and charge accumulation takes place due to an applied DC voltage$^3$. Different dielectric and flexoelectric effects become indistinguishable causing inherent difficulties in quantifying the flexoelectric coefficients.

In practice, identical responses to pulses are observed when varying the offset of a signal applied to a HAN device, implying the independence of the response from the voltage shift. Driving the device with step changes in the offset leads to either a transient increase or transient decrease in the response, depending on the polarity of the external offset. The time constant of this transient effect is consistent with the relaxation time of the ions present in the material. Assuming these ions screen out the offset effect, the remaining response can be used as a measure of the flexoelectric effect. This has also been demonstrated theoretically by adding ions into a model of the HAN cell, which reproduces this transient effect. Data and theory comparisons for transmission as a function of voltage and time allow the determination of basic device parameters such as cell thickness, the viscosity of the liquid crystal, and the ion relaxation time. Subsequent comparison between the theoretical and experimental responses of devices to pulses and changes in offset then allows the determination of the sum of flexoelectric coefficients ($e_1 + e_3$). However, this relies on the ionic screening of any offsets due to surface polarity and is therefore only applicable to materials with significant ionic content.

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Reaction-diffusion in liquid crystals

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It may be possible to carry out a reaction-diffusion process in a liquid crystalline system whereby a modulation in the concentration of reacting chemicals can affect the liquid crystalline order. This new form of active soft matter could exhibit unusual nonequilibrium structures, including Turing patterns manifest in the pseudovector or tensor field describing the liquid crystalline order and regions of opposite chirality with remarkable optical properties.
Adaptive holographic pumping of liquid crystal lasers

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A major disadvantage of organic lasers, such as liquid crystal (LC) lasers [1, 2], is the occurrence of unwanted photo-bleaching effects which can degrade and even curtail lasing output. This means that such lasers must be operated in pulsed modes at relatively low repetition rates (< kHz) [3]. This work presents an alternative pumping technique for thin-film LC lasers, which allows higher repetition rates to be accessed and photo-bleaching effects to be minimised [4].

By controlling the position of incidence of the pump beam onto LC lasers using a reconfigurable computer-generated hologram, different locations on the LC can be pumped without the need for moving parts or flushing mechanisms. It is shown that by using this technique, an increase in both the stability of the laser output with time and its average output power may be achieved.

Furthermore, by reflecting the pump laser beam from a spatial light modulator displaying a hologram that diffracts the light into a spot in a particular position – or pattern of positions – at the LC, lasing can occur from a precisely designed location or pattern of locations. This may then simply be changed by altering the hologram displayed. If the position of incidence is moved to fresh regions quickly enough, degradation effects may be minimised.

This technique also allows additional functionality such as spatial shaping of the pump beam and wavelength tuning of an LC laser, both of which are demonstrated in this presentation. Such a pumping scheme offers the potential to create novel pump-beam profiles to optimise propagation through the LC and improve the laser performance.

References:


Liquid crystal contact lenses to correct presbyopia

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The inability of the eye to focus on nearby objects, presbyopia, is suffered by \~100\% of people over the age of 50. Correcting presbyopia in contact lens users has proven elusive and existing commercial options include fundamental problems such as reduction in contrast or visual acuity. Liquid crystal lenses are subject to renewed attention, and offer to provide a compromise free method of presbyopia correction due to their ability to be turned on and off. Liquid crystal lenses are all operated \textit{via} a change in refractive index of a liquid crystal material in response to voltage application, with several different methods used to focus light, including a bulk change of refractive index of a lens shaped liquid crystal layer\textsuperscript{1}, response to a parabolic voltage distribution across a flat liquid crystal device\textsuperscript{2,3}, and various diffractive techniques\textsuperscript{4}, but have not previously been applied towards contact lens use.

We designed and fabricated a variable focus lenses for contact lens use by using a balanced optical system, which is able to provide the additional optical power presbyopes require for near vision (typically +2.00 D). The device is based on a traditional contact lens material which could be placed directly on the eye. The system uses positive optical power from the two substrates and variable negative optical power from the liquid crystal layer to form a balanced optical system which, when unpowered, corrects distance vision. Upon voltage application the liquid crystal layer decreases in refractive index, resulting in additional optical power in the system, offering correction equivalent to reading glasses. We show that the liquid crystal lens employed is well suited to the small optical areas associated with contact lenses. In addition, the influence of the liquid crystal material on optical power and operating voltages shows that focal power can be altered within the same device by a straightforward substitution of the liquid crystal material in the same device.

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Polariser free optically activated shutter

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Since 1980’s a lot of interest has been drawn to devise optical filters based on cholesteric phase for instance, notch filter\textsuperscript{1–3} colour reflector\textsuperscript{4,5} and light shutter \textsuperscript{6–8}. All of these devices utilised the unique feature of chiral nematic liquid crystals which is the well-known selective reflection band. One of the benefits of using chiral nematic LCs is that the reflection band can be “tuned” by subjecting the LC to a range of external stimuli. An active area of research is to use light to control the reflection band by using molecular structures that contain a photo-active element. This is advantageous as it offers a means of controlling the structure remotely and is particularly attractive as an optical shutter component for sensor devices. One limitation, however, is that the reflection band only exists for one handedness of circularly polarized light. Here we present a polariser free optically activated shutter based upon a short-pitch chiral nematic liquid crystal device. This device can be optically tuned as a full reflection band from 400nm to 900 nm. The LC mixture is comprised of photo-active chiral dopants, in the trans-state this device appears as a slightly yellowish in colour due to the chromophore of this photo-active component. However, as the pitch varies through exposure of visible or UV light exposure, the device becomes reflective reaching a maximum for a particular value of the pitch. As a result, it is possible to switch the device from blue to selective reflection states remotely.

\textbf{Figure}: Reversible tuning of the reflection band of the photo-responsive chiral nematic LC mixture, a) the transmission spectra showing a red-shift of the reflection band when illuminated with UV light for a period of 35 s and a power density of 5 mW/cm\textsuperscript{2} and b) The transmission spectra showing a blue-shift of the reflection band when illuminated with visible light (625 nm) with a power density of <1 mW/cm\textsuperscript{2}.

References
Multiscale models of liquid crystals dispersions of nanoparticles

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Suspension of nanoparticles in liquid crystals have been modelled on a range of scales, from molecular simulations [1] to macroscopic models [2]. 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.

Here we use homogenization theory [3] to bridge the microscopic and macroscopic scales. This method captures the underlying microscopic geometry through a series of representative cell problems derived from the underlying liquid crystal equations. These describe the local effect of a single nanoparticle on the liquid crystal alignment based on the assumption that the nanoparticles are evenly distributed and, hence, the underlying geometry is approximately periodic. By combining the results from the cell problem with the underlying microscopic equations and averaging we obtain a set of approximate macroscopic equations.

We consider two regimes of nanoparticle–liquid crystal interaction, strong and weak. In the former, characterised by high nanoparticle density and/or large anchoring energy at their surface, the nanoparticles are the dominant factor in determining the alignment of the liquid crystal.

In the weakly interacting regime, i.e. small anchoring energy and/or low concentrations, the liquid crystal director is determined by a balance between the bulk forces in the liquid crystal and the alignment at the boundary of the device and at the nanoparticles. In this regime, the macroscopic equations for the director alignment contain two key differences with respect to those for a pure liquid crystal: (i) the elastic constants are in general smaller, and (ii) there is a forcing term proportional to the anisotropy of the particles. Figure 1 shows the effect of the anisotropy on the Frederiks threshold for a 2D planar cell with elliptical nanoparticles of aspect ratio 3. As the particles are rotated with respect to the cell boundary the Frederiks threshold is shifted: even though the reduction in the elastic constant tends naturally to reduce the value of the threshold, the forcing term induced by the anisotropy of the particles can ultimately increase its value and make it larger than for a pure liquid crystal.

We discuss the derivation of these equations and the validity of the assumptions. Finally we compare the different macroscopic properties observed in the two different cases and how these equations can be used to model liquid crystal-nanoparticle suspensions capturing both the micro and macroscopic scales.

References
Cromolyn. A suitable weak NMR weak-aligning medium for small molecules

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Although it is very well known that disodium cromoglycate (cromolyn) chromonic phase\(^1\) is oriented in the presence of strong external magnetic fields, cromolyn use as an NMR alignment medium has been scarce, partly due to a too strong imparted degree of alignment. However, doping of the cromolyn solution with sodium chloride allows formation of the lyotropic phase at lower concentrations of the mesogen.\(^2\) This leads to significantly lower degrees of alignment more appropriate for the accurate extraction of residual dipolar couplings. The physical homogeneity of the N and M states of cromolyn lyotropic phases was investigated through Z-imaging 2D NMR experiments (See.\(^3\) The DSCG/NaCl system is compatible with not only neutral molecules as sugars or water-soluble norbornene derivatives but also with ionic compounds as N-methyl codeinium iodide. We tried to extend the use of the D\(_2\)O/cromolyn/NaCl system by mixing it with different cosolvents but precipitation of the phase was always observed. To our surprise cromolyn seems to show gel-behaviour in pure DMSO. The aggregation process of the mesogen in DMSO has been investigated by \(^1\)H NMR experiments.

References
New materials exhibiting non-ionic lyotropic chromonic mesophases.

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Recently, there has been an increased interest in materials exhibiting lyotropic chromonic mesophases which is being driven by emerging applications for such systems in areas including organic electronics, biosensors, micro patterned films and optical compensators as well as in the nano-fabrication of functional materials.[1] This research is at the interface between organic materials design, biomaterials, and chemical engineering. The molecular structure of such materials is based around a planar polyaromatic (plank-like or disc-like) core with polar moieties at the periphery, which, with one notable exception,[2] take the form of ionisable groups. It has been shown that the stability of the chromonic mesophases is highly sensitive to, and dependent on, the type and concentration of counterions present,[3] and hence the use of such ionisable peripheral groups somewhat complicates the understanding of the structure properties relationships.

We have designed and synthesised a new series of chromonic materials based around an elongated aromatic core, and have circumvented the need for ionic groups by incorporating flexible ethyleneoxy based chains at the periphery of the molecule as the polar group. (Figure 1)

![Figure 1](image.png)

We report here a detailed description of the design, synthesis and characterisation of these materials by DSC, OPM and XRD. We present the results of systematic structural variations in terms of their effects on phase behaviour, both as pure materials and as chromonic mixtures in water, which include nematic and higher ordered phases. Based on these results, structure properties relationships will be drawn.

References


Chromonic systems are lyotropic liquid crystal phases formed by multi-ring aromatic molecules with soluble side chains. The chromonic molecules have a strong tendency to aggregate even in very dilute solution. They aggregate face-to-face into stacks of columns forming a nematic (N) phase and, at higher concentrations, a more ordered hexagonal (M) phase. The aggregation process is often considered to be isodesmic, meaning that the energy increment associated with the addition (or removal) of a molecule to a stack does not depend on the size of the stack. Hence, the chromonic self-assembly is different to that of conventional amphiphiles, and takes place in the absence of a critical micelle concentration. Chromonic phases are formed by a range of aromatic compounds including drugs, dyes and nucleic acids.

The current molecule of interest is a 2,3,6,7,10,11-hexa-(1,4,7-trioxa-octyl)-triphenylene(TP6EO2M). The TP6EO2M molecule has discotic symmetry, consisting of a central hydrophobic core (a triphenylene ring) surrounded by six hydrophilic ethyleneoxy (EO) chains. We present and compare the simulations results for TP6EO2M aggregates in water obtained using two atomistic force-fields: GAFF and OPLS. We have analysed properties of both, the individual molecules and the stacked aggregates. Our results include calculation of (i) free energy (potential of mean force) of association of two molecules in water, (ii) distances between the molecules in the stacks, (iii) twist angle between the molecules in the stacks, (iv) bend of the stacks and (iv) hydration of the oxygens in EO chains.

The process of stack self-assembly and dynamics of aggregates will also be discussed. The comparison of our results with other simulation\(^2\) the experimental\(^3\) data will be given.

References
Most liquid crystals are organic substances which can be encouraged to show liquid crystal phase behaviour by two different approaches, either by changing the temperature or the concentration of a solvent. \(^1\) Those obtained by changing the temperature are known as thermotropic liquid crystals, and those resulting from a concentration change in solvent are termed lyotropic liquid crystals.

Liquid crystalline phase behaviour of ethylenoxy group functionalized molecules has in the main been associated with lyotropic liquid crystalline phase behaviour. For thermotropic systems it has been connected to the investigations of LC crown-ethers and for the investigation of complex perforated lamellar super-structures. \(^2\) Surprisingly not much work has been reported on the investigation of calamitic mesogens consisting of benzoic acid aromatic esters with the terminal chains bearing oligo-ethylenoxy groups. Thus such systems were explored, especially as these materials can combine thermotropic phase behaviour with some solubility in water, giving rise to the potential of chromonic properties.

In this report we describe the results of our synthetic efforts to synthesize such molecules and of the effort to attach them to gold nanoparticles (AuNPs) and of the chemical characterisation of the of the final products and the liquid crystal intermediates and the investigation of the liquid crystal properties using optical polarizing microscopy (OPM), Nuclear Magnetic resonance (1H NMR) and differential scanning calorimetry (DSC). Additionally we report our results on the qualitative miscibility studies of these molecules with water, based on OPM experiments.
Synthesis and properties of dimeric materials with lateral and terminal fluorine substituents for dual frequency liquid crystal mixtures

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Nematic liquid crystals have been widely used in electro-optical devices due to the ability to switch the orientation of materials using an external electric field. While the switching on speed can be hastened by increasing the electric field, the relaxation process is controlled by the surface anchoring energy.\[1\]

With the continuing requirement for faster switching times and alternative routes, dual frequency liquid crystal materials (DFLCs) can be found. Usually DFLC materials are a two-component mixture, positive compounds with a positive dielectric anisotropy at low frequencies and negative compounds with a large negative dielectric anisotropy that remains almost constant at different frequencies.\[1\]

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 series of dimeric materials have been targeted, these feature a core unit with lateral fluorine substituents and the other core with terminal fluorination. The aim is to synthesise materials with one core unit having positive dielectric anisotropy and the other negative dielectric anisotropy.

![Chemical structure](attachment:image.png)

The synthesis of a series of fluorinated dimers is described. With the mesomorphous properties characterised by optical polarising microscopy (OPM) and differential scanning calorimetry (DSC).

References:

The investigation of dimeric materials with a nematic – nematic phase transition

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Several hydrocarbon linked mesogenic dimers are known to exhibit an additional nematic phase (Nx) below a conventional uniaxial nematic phase (N). The correlation between molecular structure and the nematic - nematic phase transitions (N- Nx/Ntb) is not yet well understood. Nematic-nematic transitions are in thermotropic liquid crystals associated in most cases with the formation of a columnar structure in the low temperature nematic phase\(^1\,^2\,^3\) or the onset of cluster formation\(^4\) or with folding processes of polymer chains,\(^5\) there is evidence too for the formation of the twist-bend structures\(^6,\,^7\) as well as the formation of domain assemblies.\(^8\)

The synthesis of a range of such dimeric materials, symmetric as well non-symmetric systems with both positive and negative dielectric anisotropy, containing linear and bent structures in the aromatic core systems will be presented. The characterisation of these systems by the use of differential scanning calorimetry (DSC), optical polarizing microscopy (OPM) and X-ray diffraction (XRD) studies will be described in detail and the results for these systems will be compared and structure properties relationships and the impact on the formation of nematic-nematic transitions will be discussed.

References


The investigation of novel photochromic liquid crystals based on the 2,4,5-triphenyl imidazole dimer group

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In recent work a range of photochromic molecules have been used to modulate liquid crystals 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 isomerization of bonds, such as in azobenzenes, other reactions include the cyclisation in the diarylthiones or the opening of heterocyclic rings in napthopyrans. The simple cleaving of bonds by irradiation or pressure in the 2,4,5-triphenyl imidazole dimer used as a photochromic core functionalized with liquid crystal moieties has yet to be explored. The reversible change in the structure and shape of photochromic molecules has promising applications in data storage and optical drives.

In this contribution we report on our efforts in 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 cyanobiphenyl group was selected were explored in order to control the photochromic properties and the liquid crystal phase behavior. 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.

References
Graphene electrodes for liquid crystal devices in the mid-infrared


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The mid-infrared (MWIR) wavelength band stretches from 2 to 6μm and is a relatively unexplored region of the optical spectrum for liquid crystal technology. The MWIR band has many applications in both the military and civil avionics industry, as it is possible to image high temperature and intensity heat signatures such as jet engines at these wavelengths. There are now optical sources becoming available at these wavelengths, hence there is an increasing need to be able modulate and control the light. Liquid crystals have the capability to operate at these wavelengths, however there are several problems with trying to create effective devices both in terms of materials and cell construction.

One of the biggest problems in the MWIR is the choice of electrode structure as indium tin oxide (ITO) transmission drops rapidly to zero at 5μm. One solution to this is to use silicon or germanium substrates which are both transmissive in the MWIR as well as conductive, however device fabrication is quite difficult and the ability to create a pixellated structure is further limited. Another alternative is to use CaF2, which is transmissive across the visible and MWIR, but it is not conductive, hence an alternative electrode structure to ITO is required. Recent work at Manchester on graphene indicates that it is a very suitable alternative to ITO and the spectrum in Fig 1a shows that it is almost totally transparent out beyond 10μm, whist remaining conductive enough to address a liquid crystal cell.

The next challenge is then to find a suitable liquid crystal material for the MWIR. Previous work has shown that cyano based materials have characteristic absorptions at 4.1μm. Modern active matrix display materials such as TL216 have been synthesised with no cyano based groups and hence do not have this problem. This material is also desirable in the MWIR as it retains a birefringence of 0.18 at 4μm making it suitable for optical modulation. The spectra shown in Fig 1b shows a CaF2 graphene device with 20μm of TL216 being switched from 0 to 3.6V (2kHz sine wave). The upper limit on these spectra is currently the second polarisor in the system.

References
Cordite, cine film and exploding billiard balls
cellulose esters and their mesogenic properties.

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Shadowed electron micrograph of cellulose microfibrils in a plant cell wall, with a
partly-nitrated cellulose chain superimposed.

In Jules Verne’s classic science fiction novel, *From the Earth to the Moon*, it was
cellulose nitrate (i.e. guncotton) which launched the projectile into space. This exciting,
then recently-discovered material proved to be a far superior explosive to conventional
gunpowder and, as an ingredient of cordite it was manufactured in megaton quantities
during the First World War.

But cellulose nitrate had a strange range of other uses. When mixed with camphor it gave
celluloid, the first artificial thermoplastic material to be mass-produced. And for half a
century this was familiar in every household in products ranging from shirt collars to
steering wheels. Amongst its more esoteric applications, it was used as a substitute for
ivory in billiard balls. Cellulose nitrate is soluble in ether, giving a syrupy liquid called
collodion. This was widely used as a surgical dressing and, after being sensitised with
silver nitrate, it formed the working material in the ‘collodion plates’ used in early
photography.

Underlying most of the physical properties of the cellulose esters is the presence of the
straight, semi-rigid unbranched chains of the cellulose skeleton. Once the material has
been made soluble, it readily forms liquid crystalline phases, with the chirality of the
sugar units causing the phase to twist into a cholesteric state [1, 2]. Recent investigations
suggest applications of cellulose ester mesophases in electro-optical devices.

See for example:
[2] Tseng et al., Cholesteric liquid crystalline phases based on (acetoxypropyl) cellulose,
Tunable Self-Assembled Optical Metamaterials

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Liquid crystals have long been recognised as a convenient means by which to tune the plasmon resonances of various structures\textsuperscript{1}. Successful electrical, optical and thermal tuning of nanowire, nanorod, nanodisk and nanoparticle arrays, planar interfaces, and waveguides have all had their plasmon resonances tuned using liquid crystals. However, the dynamic tuning of the plasmon resonances of a fully three-dimensional structure using liquid crystals has yet to be attempted. Here we report on the use of liquid crystals to tune the localised plasmon resonances, and thereby the optical properties, of a three-dimensional optical metamaterial formed by block copolymer self-assembly.

Block copolymers consist of two or more covalently tethered and chemically distinct homopolymers or “blocks”. Due to unfavourable thermodynamic interactions between the different blocks, the copolymer melt may microphase separate, resulting in a variety of equilibrium morphologies dependent upon the type and composition of block copolymer. One such equilibrium morphology exhibits two interpenetrating and continuous regions within a third matrix region. The interpenetrating regions are triply period cubic structures of opposite handedness, termed the gyroid due to its close relation to the Schoen gyroid surface\textsuperscript{2}. Selective etching of a single block from the gyroid equilibrium morphology results in the creation of a gyroid structure template which can be back-filled with gold by electrodeposition. Removal of the remaining organic material leaves a three-dimensional gold metamaterial active in the visible regime with unit cell size of 35 or 50nm (Figure 1). The optical properties of these self-assembled metamaterials have previously been studied both theoretically and experimentally, and have been “statically” tuned by varying either the geometrical properties of the gyroid structure (e.g. the lattice constant or metal fill fraction) or the refractive index of the surrounding medium\textsuperscript{3}.

Figure 1: Fabrication of an optical metamaterial from a block copolymer. (a) Gyroid block copolymer template. (b) Selective etching of gyroid phase. (c) Metal electrodeposition. (d) Removal of polymer template.

We therefore report on the infiltration of gyroid optical metamaterials with liquid crystals, investigating the ability to dynamically tune the localised plasmonic resonances of the structure and thereby its optical properties.

References

Experimental confirmation of the Kibble-Zurek mechanism in a nematic liquid crystal.

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Topological defects appear in many aspects of physics including cosmology, superfluids and liquid crystals. The Kibble-Zurek mechanism concerns the formation of topological defects in a system driven through a continuous phase transition at a finite rate. The name was adopted after Zurek suggested that the Kibble mechanism\textsuperscript{1}, which described defect formation in the early universe, should be applicable in soft matter systems after accounting for differences in scale\textsuperscript{2}.

Predictions of how defect density scales with quench time have been made using numerical simulations but have not yet been confirmed experimentally\textsuperscript{3}. Liquid crystals can provide an experimentally accessible way in which to confirm this relationship. In this work, +/-1 defects were generated via a Fréederickzs transition in a negative dielectric nematic liquid crystal under homeotropic anchoring. The defect density was measured as the rate at which the Fréederickzs transition occurred was varied.

References
We model stable states of nematic liquid crystals confined to two-dimensional annular domains within the Oseen-Frank framework with strong, tangent anchoring on the boundary. We analyse both defect-free states and states with defects on the boundary, and consider the effects of elastic anisotropy, the ratio of the outer and inner radii and the number and arrangement of defects.

Using a combination of analytic and numerical methods, we investigate the stability of the radially invariant defect-free state. We demonstrate that this state ceases to be a global minimizer of the Oseen-Frank energy due to the effect of elastic anisotropy and describe the new energy minimizing state.

For states with defects located on the boundary, we determine the energetically preferable configuration of defects. Strong anchoring allows us to prescribe the number of defects, as well as their location and strength. Under the one constant approximation, we calculate analytic expressions for the director fields, optical textures and energies. Using finite-element methods, we are able to evaluate director fields and energies without using the one constant approximation, which we compare with our analytic results. We finally compare our results with experimental work on colloidal liquid crystals confined to annuli carried out by the Aarts group1.

References

Stretchable liquid crystalline blue phases

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The emergence of wide temperature range liquid crystalline blue phases has attracted considerable attention in recent years due to their remarkable electro-optic properties and subsequent potential in technological applications such as next-generation display devices \cite{1, 2}. Obtaining a wide-temperature blue phase can be achieved in a number of ways: for example, through the creation of a polymer network that stabilizes the defect lattice \cite{1} or through the use of bimesogenic (dimeric) compounds \cite{2}. It is well known that blue phases can exhibit photonic band gaps for visible light in three orthogonal directions, which is of importance for future technologies based upon 3-d photonic crystals (PC). Moreover, they are an example of a 3-d PC that naturally self-organises without the need for any complex fabrication procedure. Despite the numerous advances in polymer-stabilized blue phases one aspect that still remains to be demonstrated is an elastomeric blue phase, whereby the lattice structure and consequently the reflection properties can be adjusted through the application of mechanical stress. Nematic, chiral nematic, and smectic elastomers have already been studied extensively \cite{3} yet there has been no demonstration of an equivalent elastomer or stretchable gel based upon a blue phase.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure.png}
\caption{Free-standing films of a blue phase gel. The films appear coloured due to selective reflection of visible light (scale bars, 3 mm).}
\end{figure}

In this presentation, we demonstrate a polymer-stabilized blue phase I that can be stretched along a direction that is orthogonal to the plane of the film \cite{4}. This results in an extension of the lattice dimensions in the lateral directions and a contraction of the lattice parameter in the transverse direction, which is manifested as both a blue-shift in the colour of the platelets when viewed on an optical polarizing microscope and a blue-shift of the reflection band. In the latter case, the wavelength of the reflection band is found to shift by \approx 100 \text{ nm} when the stretchable blue phase is extended by 3\% in the plane of the film. To conclude, we present results on a linear electro-optic effect that only appears in distorted blue phases.

References

Phase Behaviour of Twist-Bend Nematogens

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The twist-bend nematic phase, N_{TB}, differs from a conventional chiral nematic in that the director is tilted with respect to the helix axis. In some sense the chiral smectic C phase is the smectic analogue of the twist-bend nematic phase. The existence of the N_{TB} phase was predicted by Dozov for achiral, bent-core molecules with the bent shape being an important element in the driving force for its formation [1]. The first example of the twist-bend nematic was observed for the liquid crystal dimer, CB7CB, in which two cyanobiphenyl groups are linked by a heptane spacer [2]. The spacer is flexible, allowing the dimer to undergo significant changes in its shape, indeed on average its shape is highly bent [3]. Although this qualitative feature is important in the formation of the twist-bend nematic phase the extent of the bend, that is a quantitative feature, is also central [1]. This angle in the average structure is controlled to a great extent by the nature of the link between the rod-like mesogenic group and the spacer. It appears that a methylene linking group is especially good at stabilising the twist-bend nematic phase with respect to the conventional nematic phase [2, 4]. This behaviour is also consistent with the calculation of the bend elastic constant which tends to be very small and can be negative [2, 5].

In order to help understand the phase behaviour of such nematogens we have explored the phase diagram of binary mixtures of liquid crystal dimers with odd spacers. The dimers contain terminal chains of length \( m \) as well as the flexible spacer of length \( n \). So we use the acronym \( mO.n.Om \) for these symmetric dimers. We have characterised the mesophases formed by the odd dimers using polarised optical microscopy, deuterium NMR spectroscopy and calorimetry. The spacer has a methylene link to the effective mesogenic group and the number of methylene groups, \( n \), is necessarily odd. The length of the terminal group varies from 1 to 6. The phases exhibited by some of these dimers include the expected nematic and novel twist-bend nematic. In addition, and importantly, phases with a layered structure appear as the length of the terminal chains grow; as might have been anticipated.

The binary mixtures exhibit a range of phase diagrams whose form depends in part on the commonality of the phases exhibited by the compounds. For example, when both exhibit nematic and twist-bend nematic phases the nematic-isotropic and the twist-bend nematic-nematic transitions vary continuously across the phase diagram. This shows a curious deviation from linearity. The phase diagram is more interesting when there is a not a commonality in the phases for the two components. Then phases are injected into the phase diagram as the composition changes.

References
Inkjet Printing N* Liquid Crystals onto Textile Substrates

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N* Liquid Crystals (Cholesterics) produce a wide colour gamut and provide angular colour effects that would be a welcome addition to the Textile Designer. The concept of applying structural coloured materials as opposed to conventional colouration techniques, such as dyes and pigments, has been recently explored \textsuperscript{1}. In this study, N* Liquid crystals have been applied to textile substrates using a piezoelectric inkjet printer. Solvent-based ink formulations have been deposited onto a dyed cotton substrate and have been UV-cured. Different ink formulations have been investigated and the fastness characteristics of the finished fabrics determined.

References

\textsuperscript{1}Olivier T. Picot, Mian Dai, Dirk J. Broer, Ton Peijs, and Cees W. M. Bastiaansen \textit{ACS Appl. Mater. Interfaces} (2013), 5, (15), pp7117-7121
8/2 Organosiloxane SmA–Nematic Liquid Crystal Random Lasers

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Random lasers have been an area of interest for a while now [1][2], and it has recently been demonstrated that dye doped liquid crystal (LC) materials can be used to fabricate random lasers [3][4]. One class of materials are SmA LC’s, where the electro-optic scattering behaviour is harnessed and is used to facilitate the multiple scattering of light inside the gain medium. This allows the SmA scattering domains to act as a source of feedback in a laser cavity.

In this research, we prepare dye doped (Pyrromethene 597) mixtures of 8/2 organosiloxane SmA and BL006 nematic LC with varying concentrations, in order to enhance random lasing characteristics. It is observed that the addition of BL006 results in a significant improvement in the electro-optic and lasing characteristics over the pure 8/2 SmA, and results indicate that the ideal mixture concentration is around 40 % SmA, 60 % BL006.

We show that in addition to an increase in thermal stability of the mixtures over the pure 8/2 samples, the addition of a nematic leads to faster response times, lower electric field thresholds, lower laser pump thresholds and narrower emission bandwidth.

Device lifetimes are also studied, and it is found that CTAB doped SmA-N mixtures are unstable for long term operation under the application of electric fields. To increase lifetime, we add redox dopants Tetracyanoquinodimethane (TCNQ) and Phenylene diamine (PDA), and investigate random lasing under both dynamic and static scattering conditions. Results summarizing the difference in lasing characteristics of the different concentration mixtures are shown, Figure 1.

Figure 1 (a) Laser threshold energies plotted against frequency for all the mixture, clearly there is a significant effect on laser threshold with changing mixture concentrations. (b) Represents the variation of the FWHM (full width half maximum) with the input pump pulse energy of the source at an applied electric field frequency of 100Hz used to induce electro hydro-dynamic (EHD) scattering

References

Computer simulations of an anionic chromonic dye: spontaneous symmetry breaking to form chiral aggregates and the formation of a novel smectic phase

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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 right). 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.

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 self-assembled aggregates and phases.

Results for low concentration systems show a spontaneous symmetry breaking wherein chiral aggregates (see figure left) form as the energetically most stable species, despite the presence of strictly achiral dye molecules. This provides a new interpretation of experimental results.

Results for higher concentrations show the alignment of several aggregates to form a novel smectic layer structure, with the inherent loss of chirality as a result of this new molecular environment. The formation of the novel layer structure, which is stabilized by interactions of surface charged groups, as well as the biaxial nature of the structure formed, explains the key experimental findings.

Hence, the simulation results point to the formation of a hitherto unknown smectic chromonic mesophase.

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Constructing a Fourier optical derivative coprocessor

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The idea of coherent optical information processing using the Fourier transforming property of a simple lens is an old one,\textsuperscript{1} and exploitation of the fact that differentiation reduces to multiplication in the Fourier domain was suggested a long time ago.\textsuperscript{2,3} Recently, implementations using metamaterials have been proposed.\textsuperscript{4} However, no successful system has been built to viably implement this concept. Such a system could potentially offer a step-change in capability for performing simulations which rely heavily on differentiation, such as fluid mechanics. For example, an 8K×8K differentiation can take over 100 ms on a supercomputer, but could be accomplished in less than 1 ms in the optical domain if high refresh rate analogue ferroelectric liquid crystal SLMs were used for the input.\textsuperscript{5} The inherently parallel nature of diffractive optical computing means that the computation time does not scale with the size of the problem. Furthermore, an optical system has the potential to be significantly more energy efficient.

This work will explore the engineering challenges to implementing a differentiating coprocessor system in a 4f-architecture similar to a matched filter optical correlator.\textsuperscript{1} A synthetic VanderLugt filter to encode the complex filter as an amplitude-only filter is explored, and the viability of expressing this filter on a SLM is considered. Further, a technique to mitigate the inherent pixelation and artifacts associated with displaying an image on an SLM through a controlled blurring using a Gaussian Fourier plane filter is presented.

The 4f-system architecture and the corresponding amplitude and phase components of the filters required for first and second order differentiation.

References


Flexoelectricity and flexodomains in a bent-core oxadiazole nematic liquid crystal

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Bent-core nematic liquid crystals (NLC) are exciting materials exhibiting unusual elastic constants, anomalous electroconvection (EC), reports of biaxiality, ferroelectric properties and giant flexoelectric coefficients.1 Many of these possibilities are still hotly debated. Our recent work on Frank elastic constants in oxadiazole and thiadiazole based bent-core NLCs proved that what was considered unusual behavior of these materials in terms of elastic behavior could be explained fully from considerations of their molecular structure.2,3,4

The flexoelectric coefficients of the bent-core materials are highly controversial. Indeed, there are only a few reports of values in bent-core materials, mostly at a single temperature or a narrow range, and none across the complete temperature range of the nematic phase in a bent-core material. Therefore, in this paper; we report a study of the temperature dependence of flexoelectric coefficients determined for an oxadiazole bent-core LC across the complete 60 K wide nematic regime. Measurements of $|e_1 - e_3|$ are deduced using the critical voltage for formation of flexodomains and their wavenumber, together with the elastic constants and the dielectric anisotropy. The coefficients $e_1$ and $e_3$ are also calculated using a computational methodology based on a molecular field approach with atomistic modelling and compared with the experimental values. Our data show large (tens of pC), but not giant magnitude of the coefficients and the value increases with reducing temperature. Flexoelectricity, which was discovered in LCs more than four decades ago, has recently been in the limelight because of its potential application to actuators, sensors and energy harvesters. Understanding the bent-core systems and their unusual properties is the key to their future use.

References:

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A simple model for the aggregation of chromonic molecules

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Chromonic mesogens are non-conventional amphiphiles, which self-assemble in aqueous solution to form aggregate structures: rods, stacks or layers. These aggregates can subsequently self-organise 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. The driving force for chromonic aggregation is hotly debated. For different chromonic systems, static charges, polar and quadrupolar interactions, microphase segregation and entropic contributions to the hydrophobic effect have all been claimed to be significant.

In this poster we show that a chromonic molecule can be represented by a disk with attractive and repulsive areas of interaction to mimic the attractive forces during aggregation. Simplifying a molecule in this manner allows for the reproduction of many of the aggregation properties seen in real chromonics; explaining the variation of binding with concentration and the formation of helically ordered aggregates.

The shape of the disks can be distorted to better represent specific molecules, demonstrating how small changes in chemical structure can lead to dramatic differences in aggregation behaviour. Results from this simple model show a remarkable agreement with the predictions from atomistic simulation studies of chromonic disks in aqueous solution.

Figure 1: The interaction between two circular chromonic molecules can be represented as a series of overlaps of attractive and repulsive regions of two disks. Using these overlaps we can predict the most favourable stacking configuration and demonstrate how small chemical changes are reflected in changes in aggregation.

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Using liquid crystals to induce order in an array of gold nanoparticles: a simulation study

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Experimental studies have established that anchoring a variety of liquid crystal ligands to metallic nanoparticles can lead to the self assembly of the nanoparticles into a variety of ordered geometries\(^1\). Being able to control such structures is of great interest in electronic, optical and photonic applications, ranging from negative refractive index cloaking devices to plasmon waveguides and band pass filters.

Despite much experimental work being performed on these systems to synthesise and characterise the ordered phases produced, they are yet to be well understood. The main aim of this work is to use dissipative particle dynamics (DPD) simulation to gain a molecular-level insight into the factors dictating phase formation in this system. For instance, it has been proposed by Mehl et al.\(^1\) that the organic corona surrounding the nanoparticles deforms under certain conditions, leading to the formation of a cake-like shaped unit. These units then stack to form a hexagonal structure, as illustrated to the right. We hope that our work in simulating these superparticles can either validate these proposed mechanisms, or put forward the basis of an alternative.

To date, most experimental success has been found by laterally attaching a nematic-phase forming liquid crystal to the surface of gold nanoparticles, details of which are illustrated to the left. We have produced a coarse grained representation of these superparticles, in order to take advantage of DPDs ability to simulate on the mesoscale (rather than be limited to much smaller scales in using traditional molecular dynamics).

By considering a variety of distinctive properties of the superparticles, we hope to establish which variables are most important in affecting their phase behaviour, and how these can be best tuned to produce the favoured nanoparticle arrangement for any particular application. This level of control over the order of the nanoparticles would allow for extensive engineering of novel optoelectronic materials, allowing significant progress in the area of photonics.


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Synthesis and investigation of gold nanoparticle grafted liquid crystalline polymeric nanocomposites

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Research into gold nanoparticles coated with rod-like mesogens has attracted a considerable degree of interest in the last few years, due to their unique property of self-assembly into 1D, 2D and 3D nanostructures. The self-organizing ability of the liquid crystal molecules forming the coating around nanoparticles (acting as central scaffolds) has been to be the driving force for the self-assembly of nanoparticles into 3D superstructures with optical properties that are potentially new class of stable liquid-crystalline metamaterials.

The structure of superlattices formed by nanoparticles and the values of lattice parameters can be achieved by careful selecting and controlling the size of the nanoparticles and there is the promise of interesting plasmonic properties. A parameter which has been investigated in less detail is the size of the organic corona. Here we present our results on the investigation of gold NPs were side-chain LC polymer chains (SCLCPs) have been attached to the NPs, with varying length of the chains and the number of mesogenic groups. The preparations of SCLCPs, either by grafting to the NPs or by polymerisation from by the preparation of an Au-NP macroinitiator, were explored. The mode of polymerisation either free radical polymerisation or atom transfer radical polymerisation (ATRP) was varied.

The results of the synthetic work will be presented and the chemical characterisation by NMR, GPC and MALDI-TOF and TEM of the AuNP-SCLCP nanocomposites will be reported. Optimized design pathways towards such systems will identified, having in view a focus on the size of the NPs and the molecular weights of the SCLC polymer chains. The results of the LC properties of these systems, based on OPM, DSC and XRD investigations will be reported. The properties of these systems will be discussed and will be compared to structurally related materials.
Tunable multi-functional nanostructured holograms using liquid crystals

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Holography is an important optical technique that records information on both the phase and amplitude of light and can therefore be used for 3D image reconstruction. Enabling true 3D digital holography requires the control and modulation of a range of the properties of the incident light. Liquid crystal based technologies, such as spatial light modulators (SLMs) are the most common route to achieve holographic reconstruction [1]. Ideally every pixel in such a display should modulate independently various properties of the optical wavefront, e.g. its phase, amplitude, polarisation. The wavelength-dependent nature of holography greatly increases the difficulty of this task.

Here we employ metallic nanostructures and liquid crystals to enhance the functionality of standard multi-colour liquid crystal pixel. By tailoring the sub-wavelength dimensions of such metallic nanostructures, sharp wavelength-dependant plasmon resonances can be achieved which are detectable in the far field [2]. Using these structures as the fundamental scattering element, we have been able to spatially multiplex together two wavelength- and polarisation-dependant intensity holograms as shown in Figure (a) [3]. Therefore control of the hologram’s replay field, shown in Figure (b), is achieved by adjusting the incident polarisation of light and multi-colour holography is realised using the wavelength dependant resonances of the nanostructure scatterers. Using these structures on the silicon backplane of a typical liquid crystal cell, we have shown multi-functional modulation of the replay field and hence output of the pixel is possible through the applied bias of the cell and hence the switching of the liquid crystal orientation.

References


Aggregation behaviour of aqueous solutions of the azo dye Acid Red 266: MD simulation study

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The azo dye Acid Red 266 known as Nylomine, is a disparate ionic dye that forms chromonic mesophases at unusually low concentrations (0.25% (w/w))1. Nylomine exhibits a nematic tiger-skin texture at 1% (w/w) and does not show a sharp N/M transition2,3. Despite the low concentration, the Nylomine aggregates have a cross sectional area far larger than the molecular area. In an attempt to gain insight into aggregation behaviour of Nylomine and the structure of this chromonic mesophase, we carried out molecular dynamics simulation in water and in mixture of Sunset Yellow dye. The binding energy of Nylomine dimer was estimated from steered MD simulation. It is unclear whether the fundamental building block for supramolecular assembly is a Nylomine dimer or a larger aggregate species.

References
Optimisation of force fields to describe liquid crystal molecules: the path to a dramatic improvement in \textit{ab initio} transition temperature prediction

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Computer simulation, using a range of models from coarse-grained to fully atomistic, provides a powerful tool for investigating liquid crystalline materials. Although coarse-grained models have the advantage of being suitable for the study of large systems at reduced computational cost, fully atomistic simulations have the potential to link chemical details with the properties of a system. For example, the phase transition and stability of particular mesophases are known to be extremely sensitive to small changes in chemical environment.

However, the phase diagram and mesophase properties derived from atomistic simulations strongly depend on the force field (i.e. the model) employed and its description of the molecular geometry and intermolecular interactions. The current generation of chemical force fields has not been accurate enough to provide reliable predictions of transition temperatures for many liquid crystals.

\begin{center}
\textit{Left: The structure of the nematogen 1,3-benzenedicarboxylic acid,1,3-bis(4-butylphenyl)ester. The new force field predicts the nematic-isotropic clearing point to within 5-10°C (an improvement of 55°C) over a standard (GAFF) force field.}
\end{center}

This paper presents results from an optimisation study of the model force fields used to describe liquid crystal molecules at an atomistic level. We show that with careful optimisation of the parameters describing liquid crystal fragment molecules, we are now able to make \textit{ab initio} predictions for nematic mesophase formation, and predict the N\textit{\rightarrow}I transition temperature within 5-10°C. This is a huge improvement over the state-of-the-art from just a few years ago, and suggests that, in the future, atomistic simulation will become a valuable tool to predict mesophase behaviour prior to synthesis.
Graphene LC devices

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Graphene is a single atomic layer material which has been well recognized in the form of a transparent conductive layer and found to be an ideal alternative to thin layer metallic or metal-oxide conductors. Liquid crystals (LC) have been found to be instrumental in visualizing large (\(1\)\(\mu\)m) area graphene (Gr) domains by imaging the birefringence of a Gr surface covered with nematic liquid crystal molecules \cite{Kim et al. 2012}.

In this work we present the study of the alignment phenomenon of a Gr with nematic (5CB), smectic (11CB) and chiral LCs and the possibility of using Gr as a transparent electrode layer in electro-optical devices. Transparent and conductive films (TCF) play an essential role in modern electro-optical devices \cite{Phillips et al. 1994}. These conductive layers or electrodes are usually provided by a thin transparent layer of metal (e.g. Au, Ag) or in the form of a thin layer metal oxide. In current LC devices indium tin oxide (ITO) is usually used as a TCE and Polyimide as a molecular alignment layer. However, currently there are several issues associated with the use of these thin metal oxide films, such as the need for antireflection coating \cite{Phillips et al. 1994}, non-uniform absorption of the layers across the visible spectrum \cite{Phills et al. 1994} and chemical instability \cite{Schiltheim et al. 2008}.

In contrast, Gr is a two dimensional optically transparent material with high crystallographic quality \cite{Meyer et al. 2007} which also exhibits a high Young’s modulus \cite{Nair et al. 2008}. It is therefore a good alternative to ITO. In addition, polycrystalline Gr possesses random domain orientation which enables the liquid crystal molecules to align according to directors within the domains. This additional feature of Gr together with its conductive characteristic makes it possible for it to be used as a transparent electrode and alignment layer in electro-optical devices.

![Graphene LC devices](Image)

**Fig 1:** Optical micrographs under crossed polarizers. Optical visibility of graphene domains and study of the alignment phenomenon with different types of LC. (a) nematic 5CB; (b) smectic 11CB; (c) chiral; (d-f) transmission vs applied electric field optical micrographs for Gr-ITO cell. Nematic LC 5CB is used as an optical medium, (d) no electric field applied (e) under applied electric field 5V/\(\mu\)m, 1 kHz (f) under applied electric field 10V/\(\mu\)m, 1 kHz.

Reference

Synthesis and Properties of Novel Liquid Crystal Materials with Bulky Terminal Chain for Ferroelectric Display

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Difluoroterphenyls\textsuperscript{1} are well-recognised as excellent host materials for low viscosity, fast-switching ferroelectric mixtures. Ferroelectric liquid crystal displays switch faster than conventional liquid crystal displays, and offer much higher resolution, and hence are suitable for microdisplay applications\textsuperscript{2}.

\begin{center}
\begin{tikzpicture}
\node at (0,0) {a, b, c, d, e and f = F};
\end{tikzpicture}
\end{center}

The synthesis and mesomorphic properties of a systematic range of ortho difluoroterphenyls and ortho difluoroquartetphenyls with bulky terminal chains are detailed. The bulky terminal chain consists of a methoxy-4,4-dimethylpentyl group, a trimethylsilyl unit and a dimethylethyl group. All the final products will be evaluated for their mesomorphic properties and a wide range of other physical properties, and the most suitable compounds will be formulated into mixtures for evaluation in prototype microdisplays. Some of those compounds give a nematic phase however, all the compounds give a SmC phase.

References

Synthesis, Mesomorphic Behaviour and Optical Anisotropy of Some Novel Liquid Crystals with a 2,6-Disubstituted Naphthalene Core and Lateral Fluoro Substituents

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The variety of liquid crystals that find commercial applications is currently very wide. Nematic liquid crystals dominate commercial applications in displays, and several different device formats are available, for example twisted nematic (TN), super-twisted nematic (STN), in-plane switching (IPS) and vertically-aligned nematic (VAN), that require materials of differing specific properties.\(^1\) Ferroelectric liquid crystal displays (FLCD) require smectic C materials with properties tailored for the specific application.\(^2\) Chiral nematic liquid crystals selectively reflect visible light of a wavelength that depends on temperature, and hence find extensive use in a wide range of commercial applications most notably thin-film thermometers, document security logos and specialist paints and coatings. In all such applications the need for high optical anisotropy (birefringence)\(^3\) is increasingly important, for example in displays to allow the advantageous use of thinner cells, and in thermochromatic applications to generate an acceptably high brightness. In addition, high optical anisotropy is an essential feature of nematic liquid crystals intended for telecommunications devices, particularly those operating at 1550 nm.

Unfortunately, many structural units conducive towards a high optical anisotropy cause a high melting point, high viscosity, low solubility, low resistivity and low chemical and photochemical stability, features which are incompatible with the materials used in commercial applications. The synthesis, mesomorphic properties and optical anisotropy of a range of fluorinated diphenylnaphthalenes with a terminal pentyl or butoxy chain (1a-c) are detailed. The design of the materials serves to combine high optical anisotropy, through the use of a naphthalene ring and two benzene rings, with a low viscosity, high resistivity and compatibility with existing commercial materials by maintaining a fluoro-hydrocarbon structure. The synthesis of the materials was effected efficiently using a combination of low temperature lithiations and Suzuki couplings. The materials exhibit very high nematic phase stability, as determined by optical polarizing microscopy and differential scanning calorimetry. As expected, the optical anisotropy of all the materials is high with values in excess of 0.3 at 25 °C, as measured by refractometry through extrapolation of mixtures in a commercial mixture of low optical anisotropy.


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Design and Study of Gold(I) Containing Liquid Crystals

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Metal-containing mesogens have attracted interest due to their ability to form tailored structures suitable for column stacking and in addition to promote interesting properties related to the incorporated metal atoms into liquid crystalline materials. Metallomesogens which contain several metals have been reported in the last years; however relatively few gold-containing mesogens exist in literature. Even less reported are the examples of trinuclear gold containing liquid crystals. Notable exceptions are the works on pyrazolato complexes for which hexagonal columnar mesophase behaviour was detected near room-temperature. [1-3] Conceptually related are the planar pyridine based gold complexes first reported in the 70’s [4,5] where the planarity of the structure was confirmed [6]. These compounds are very promising targets for exploring the nanostructuring of gold(I) in organic matrices.

In this contribution we report on the synthetic pathway followed for the preparation of the liquid crystal (Au-pyridine)₃-Rₓ substructures. The trinuclear metallomesogens studied herein have the general structure shown in Fig. 1, where the length of the terminal alkyl chain was varied between six and fourteen hydrocarbon atoms. The nine-membered ring involves three two-coordinated Au atoms and its properties arising from the attractive aurophilic interactions. We will report on our synthetic efforts and characterization of these materials. The results of our OPM, DSC and temperature dependent XRD studies, including GISAX studies will be presented. Correlations between structure and arrangements of the molecules in the liquid crystalline phase will be made.

Figure 1: (left) structure of the investigated system [C14-PyAu]₃; (right) electron density map of [C14-PyAu]₃ in the columnar phase with a schematic molecular model overlaid on top

References
Synthesis and Investigation of dimeric liquid crystal molecules with nematic-nematic phase transition

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The occurrence of a nematic-nematic phase transition is one of the unusual properties which were recently noticed in the investigations of organic liquid crystals. Such a transition has been seen initially in the investigation of dimeric liquid crystals with cyanobiphenyl based mesogens separated by a hydrocarbon spacer consisting of an odd number of methylene groups. Since the first report of such materials similar behaviour has been detected in a number of chemical architectures and phase transitions in bent-core systems and of LC polymers could be associated to similar behaviour. In this report we will describe the results of our synthetic efforts of modulating the spacer structure of LC dimers using a cyanobiphenyl mesogenic core and of the chemical characterisation (NMR) of the materials and the investigation of the liquid crystal properties using optical polarizing microscopy (OPM) and differential scanning calorimetry and we discuss the structure properties relationships.
Nematic mixtures of rods and discs - synthesis and investigation

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From theoretical studies, it has been proposed that the biaxial nematic phase may occur in mixtures of disc-shaped and rod-shaped particles. Conceptually the clearest approach is to mix discotic and calamitic mesogens in the nematic phase. Although mixing of both moieties in the nematic phase is not prohibited for symmetry reasons (both materials show a uniaxial nematic mesophase), stable mixtures of rods and discs are very difficult to prepare and most approaches have so far relied on connecting disc and rod shaped molecules covalently. The aim of our work is to study the miscibility of non-covalently linked nematic rods and discs. To this end, we chose the pentaalkynylbenzene motif \(^1\) (eg 1) for the disc component and have designed and synthesised novel discogens which exhibit only nematic mesophase behaviour.

The recent report that multiynyl thiophenes can exhibit mesomorphic behaviour encouraged us to explore these materials further \(^4\) and we have recently reported a new series of nematic only mesogens based around tri- and tetra-ynyl thiophene cores substituted with alkoxy naphthalene units such as \(^2\), and these compounds form the rod component of the mixtures. A systematic investigation into the miscibility of these rod-like and disc-like molecules in the nematic phase has found that a wide range of these materials are indeed miscible. Here we present the results of this work, including the molecular design, synthesis and mixing behaviour, including analysis of the nematic mixtures by DSC and OPM and phase diagrams of the nematic mixtures will be presented.

References

The synthesis and investigation of novel photochromic liquid crystals based on functionalized diazocines

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The modulation of liquid crystal properties by the introduction of photochromic groups has been widely investigated. The main group investigated for this effect is azobenzene group, however there are also other molecular architectures that have been explored such as naphthopyrans, diarylethenes and spyropyrans. [1] The photochromic properties of diazocines, [2] where the most stable conformer of the molecule is the cis conformer has not been investigated to any large extend. Interestingly when irradiated these class of molecules isomers to the trans form, which forms two states the twist or less favoured chair conformation, have yet to be investigated for the effects on the liquid crystal phase. This class of materials sows potential for generating photoactive LCs, where irradiation induces LC behaviour or enhances the stability of the LC state.

In this contribution we will report the design and the synthesis of a novel range of systems with these so far uninvestigated photochromic groups linked with liquid crystal moiety. The design features such as hydrocarbon spacers between the liquid crystal moiety and the photochromic core along with the direct attachment of extended partially fluorinated aromatic liquid crystal groups to the core, the effect on the liquid crystal properties will be discussed. The photochromic and liquid crystal properties will be investigated and the liquid crystal properties will be analyzed by OPM, DSC and XRD. The affects of the attachment of the liquid crystal group to the photochromic core such as the photochromic properties and the liquid crystal phase behaviour will be discussed.

References

A simple mono-hydroxyalkyl substituted cholesterol liquid crystal

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The first liquid crystal was a derivative of cholesterol and the same mesogenic unit has since been employed in a myriad of molecular designs to produce liquid crystalline behaviour. We report a very simple modification, the addition of an alkyl chain with a terminal hydroxyl group (Figure 1). The inclusion of polar groups such as a diol, or carboxylic acid can produce complex self-organising behaviour. In these examples, even a single hydroxyalkyl group provides sufficient intermolecular hydrogen bonding to give liquid crystalline behaviour presumably with a degree of microphase segregation. The developments in this area and in chromonics continues to blur the boundaries between lyotropic and thermotropic liquid crystals.

![A simple hydroxyalkylcholesterol showing liquid crystalline behaviour](image)

A simple hydroxyalkylcholesterol showing liquid crystalline behaviour

*Figure 1*

References


Evaluation and molecular modeling of chiral dopants for ferroelectric liquid crystals

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The demand for high definition displays and the development of RGB sequential illumination of pixels demands faster switching speeds than can be achieved by conventional nematic technology. OLED and blue phase displays are alternatives that may fulfill all the device requirements but ferroelectric liquid crystal displays (FLCDs) are a proven alternative. The alignment problems of FLCDs has been it’s Achilles heel and material development is one area that can improve alignment behaviour.

The chiral dopant is an important component of an FLC mixture. Novel mesogenic and non mesogenic optically active cyano ether linked chiral dopants with different chiral centres with fluorinated bi- and ter-phenyl core units have been designed and synthesised. Phase transitions, spontaneous polarisation, switching cone angle and optical textures of the chiral dopants in different compositions with the achiral FLC host mixture KCHM211 are investigated. The helical twisting powers of the mixtures are determined by using The Cano wedge method. The spontaneous polarisations of the mixtures are lower than expected and we try to rationalise this using molecular modelling. The modelling derived geometry is compared with that from single crystal X-ray diffraction.

Figure 1: Ether linked FLC dopant structures and the geometry obtained from single crystal X-ray diffraction

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References


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All-optical method for measuring the time response of nematic liquid crystals

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Knowing the time response of a liquid crystalline material is of great importance when designing a liquid crystal device. Numerous methods exist for measuring the rotational viscosity ($\gamma_1$) of a liquid crystal\textsuperscript{1}, which can in turn be used to calculate the so-called rise and fall times of the material using e.g. the equation $\tau_{\text{eff}} = \frac{d^2 \gamma_1}{K_1 \pi^2}$ for the fall time in the splay geometry, where $d$ denotes the thickness and $K_1$ the splay elastic constant.

We present a new, all-optical technique to measure the rotational viscosity of nematic liquid crystals in a planar geometry. The technique is based on common phase-lag measurements of light passing through a cell placed between crossed polarisers with an applied electric field (figure 1), and therefore does not require bespoke equipment. Other advantages to this method are that it does not measure transient behaviour that can be significantly affected by initial conditions, and it is possible to concurrently extract other important liquid crystal parameters such as the birefringence, elastic constants $K_1$ and $K_3$, Friedericksz transition and pre-tilt.

A 500 Hz AC field is applied to the cell, and the output intensity is measured as a function of amplitude. The liquid crystal responds to the RMS of this field, while at the same time undergoing small oscillations at twice the frequency. The mean data can be fitted using a standard free energy model in order to extract the aforementioned static parameters, while Erickson-Le Leslie theory\textsuperscript{2} allows us to fit to three characteristic Leslie coefficients, including $\gamma_1$.

Figure 2 shows the fitted data for both the range and mean (insert) of the measured intensity for E7. We have found that the measured rotational viscosity matches up well with literature values for E7, TL205 and ZLI792 (Merck), and that the method is more reliable with thinner cells. We are now calculating the accuracy of this method, and hope that it will prove to be a useful and powerful tool for any liquid crystal scientist investigating new materials.

![Figure 1: Measuring director orientation of a liquid crystal cell between crossed polarisers](image1.png)

![Figure 2: Fitted experimental data](image2.png)

References

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Optical diffraction experiments are often hampered by the presence of speckle, which appears across the image plane as a high contrast granular pattern\textsuperscript{12}. This speckle reduces the resolvable feature size and increases noise of the optical system\textsuperscript{1} as shown in the checkerboard image. This can make analysis and post processing of results difficult\textsuperscript{3}. Despite uniform illumination, when the signal is coherent and complex, speckle always arises due to the stochastic properties of the system\textsuperscript{1}. There are many methods used to reduce speckle including motion of a diffuser or deformable mirror and time-averaging over multiple wavelengths, orthogonal polarizations, or diffraction patterns with additive noise\textsuperscript{123}. All these methods work to either reduce speckle by controlling spatial or temporal coherence or by performing spatial sampling or averaging with varying effect\textsuperscript{3}. We examine the effects of transmissive smectic liquid crystal devices in the reduction of speckle, as well as the effect when combined with other methods.

References
Disk-like (discotic, columnar) liquid crystals were discovered in 1977 by Chandrasekhar et al.. They offer novel applications as a result of their orientations in columnar mesophases. The significant applications of the discotic liquid crystals are the negative birefringent films to wider the viewing angle on displays and the lubricants on hard-disk drives in computers.

Miscibility is a powerful tool in the study of liquid crystals and for the confirmation of mesophase types. In calamitic systems miscibility and the use of Gibbs phase diagrams is commonplace, and has led to the formation of eutectic mixtures for wide operating temperature materials for displays. The liquid crystal mixtures were created to lower the melting point of liquid crystal materials, to increase the liquid crystal phase range, or to improve upon the electronic capability. Classically, binary and more complex liquid crystal mixtures were prepared using the Schröder-Van-Laar equation to lower the melting point of liquid crystal materials through the formation of eutectic mixtures, and to increase the liquid crystal phase range for wider operating windows for display applications. For discotic liquid crystals, however, this is not the case.

The miscibility of discotic liquid crystals of differing core structure has been investigated. These studies included mixing materials such as symmetric triphenylene hexa-esters, phenyl hexa-alkynes, and new asymmetric tiphenylene hexa-ethers (Figure 1), which exhibit the same or different mesophase with respect to each other. Structure-property correlations were formulated and eutectic mixtures based on Gibbs phase diagrams are reported and discussed. These studies show that discotic liquid crystals are not necessarily miscible with each other, unlike classical nematic or smectic liquid crystals and hence might be classified as soft crystal phases.

![Figure 1](image-url) One of the structures of new asymmetric triphenylene hexa-ethers.

References

“Chess-board” based 2D and 3D LC phases of X-shaped polyphiles

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The self-assembled liquid crystal structures observed in X-shaped molecules have attracted much attention owing to their diverse morphologies and potential applications. Most prominent are a series of LC honeycombs with cells of different polygonal shapes. Among them is a square honeycomb displayed by X-shaped polyphiles. The present X-shaped polyphilic molecule Si5F10 consists of a rigid rod-like aromatic core with a carbosilane and a semiperfluorinated alkyl chain attached laterally to opposite sides of the aromatic moiety. Small-angle X-ray scattering is used to determine the structure at different temperatures. Si5F10 forms 3 different LC phases in the temperature range between 86 °C and 130 °C. The high temperature phase can be indexed on a square 2D lattice, while the middle and low temperature phases can be indexed on a body centred tetragonal and a primitive tetragonal 3D lattice, respectively. In the high temperature phase, the lattice parameter a is about $\sqrt{2}$ times the length of the aromatic rod, while in the middle and low temperature phases, a is about twice the rod length. This, combined with the electron density maps, suggests that the aromatic moieties form a chessboard-like square honeycomb net with carbosilane and semiperfluorinated chains filling the alternative “chessboard” cells. On cooling, the shrinking carbosilane columns condense into rows of periodic discrete “droplets”, creating modulation in the 3rd dimension – see Figure. The 2D-3D transition is also accompanied by reorientation of rod-like aromatic cores.

References
**Superlattice in Dendron-Alkane mixtures**

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Wedge-shaped mesogens with flexible pendant chains often assemble in thermotropic columnar or cubic phases. For wedge-shaped alkali metal 3,4,5–trialkoxybenzoate salts (“minidendrons”) columns and spherical “micelles” in the cubic phases were found to shrink in diameter dramatically with increasing temperature.\(^1\) This was explained by the wedge widening as the alkyl chains expand laterally due to increased conformational disorder. In turn this leads to exclusion of excess dendrons from a column or micelle and their reassembly in new smaller columns/micelles. The exceptions are the salts of lithium, where the columnar diameter stays constant with increasing temperature, in fact increases slightly.

In recent experiments we prepared a series of mixtures of Li 3,4,5–tridodecyloxybenzoate with n-alkanes and observes the formation of a hexagonal superlattice (Col-s) at the high-temperature end of the Col-h range. The supercell contains 3 columns. Electron density maps based on XRD suggested that two of these contain 4 molecules within the column cross-section (stratum), while the third contains only three. Interestingly, the transition to the superlattice allow the average column diameter to shrink, an option apparently denied by the Col-h phase.

To understand the superlattice, we replaced the n-alkane with a perdeuterated one (n-C\(_{19}\)D\(_{40}\)) and performed temperature-dependent neutron diffraction experiments. Figs. 1a,b show the diffractograms of the Col-h and Col-s phases, respectively. The scattering length density (SLD) map of the superlattice, reconstructed from the intensities in Fig 1b, is shown in Fig 1c. The highest SLD “bow-ties” represent the alkane-rich regions, the high-SLD column centres are the aromatic regions and the low-density rings are the hydrogenous alkyl tails of the minidendrons. What the map tells us is that of the three columns in the supercell, one two has 4 dendrons while the third has only one. However to the outside the 3-dendron columns appear the same size as the 4-dendron columns, since the free alkane aggregates preferentially in and around the 3-dendron columns making up for the shortfall in their volume. This way the lattice strain that would arise from packing of unequal columns has been alleviated.

Left: SAXS and SANS powder patterns of the Col-s superlattice in the minidendrons + n-C\(_{19}\)D\(_{40}\) mixture. Right: Neutron scattering length density map of Col-s phase. Schematic: white triangles = minidendrons; OO = alkane.

Channeled-layer LC phase in cylindrical confinement

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Geometric confinement has significant effect on the phase behaviour and orientation of LCs. Here we study the so-called channeled-layer phase (ChL\textsuperscript{1}) of T-shaped facial amphiphiles confined in 400 nm cylindrical pores in anodized aluminium oxide as well as in a 2.5 µ diameter glass capillary. The ChL phase has 3D order and consists of alternating aromatic and aliphatic layers with a hexagonal array of polar channels cutting through the stack normal to the layers. The influence of the size of the pores and the cooling rate on molecular orientation was investigated by small-angle X-ray scattering. In nano pores the order of the polar channels is partially lost and a smectic phase is induced. The orientation of the ChL phase depends strongly on the cooling rate from isotropic. It was found that under fast cooling the columns in the ChL phase orient perpendicular to the long axis of the pores due to their homeotropic anchoring on the walls, while under slow cooling the columns are parallel to the axis. Nucleation vs. stability in directing alignment of confined 3D LC phases is discussed.

Figure. Molecular structure of the T-shaped amphiphile and the sketch of the ChL\textsubscript{hex} phase.

References
The self Assembly of CdS Quantum Dots with Dendrimeric Mesogens:

Cubic with a Twist!

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Materials comprising organised arrays of quantum dots (semi-conducting nano-particles) possess a great technological significance due to their interesting optoelectronic properties; hence their potential, or current application, within a variety of nanoscale devices. The self assembly of nano-particle arrays through dendrimeric mesogen grafting has already been documented, however they show that the assembly is limited to basic arrangements such as body-centred cubic [1] or simple cubic [2]. Here we present a complex cubic formation of cadmium sulphide (CdS) quantum dots, facilitated by the attached phenethyl-ether type dendrons (shown left). This new phase of mesogenic self assembly was determined through grazing incidence small angle x-ray scattering (GISAXS) of a thin film (annealed in chloroform vapour at 150C), as well as volume fraction conversions from thermogravimetric (TG) analyses. These procedures revealed systematic absences of the hkl peaks (100) and (300) consistent with the reflection conditions 00l=2n, and a unit cell (a=11.8nm) containing four CdS nano-particles. The results, and the good match between observed and simulated diffraction intensities (to within 3%), indicate a structure described by spacegroup P2_13…cubic with a twist! This interesting result shows the possibility of complex self assembly within particle-dendrimer systems and perhaps the presence of induced chirality; this in turn may add further variety to the local interactions, hence optoelectronic properties, achievable within quantum dot arrays.

References


Synthesis of Dihydroazulene Photoswitches with Liquid Crystalline Properties

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Dihydroazulene (DHA) is a photoswitch where a ring opening reaction can be facilitated by light to afford vinylheptafulvene (VHF) which is coupled with a thermally driven back reaction.\textsuperscript{1} Recent advances have allowed for the synthesis of DHAs with substituents in both positions 2 and 7.\textsuperscript{2} Our research interest is geared towards using the newly developed methodology to strategically place alkyl bearing groups at opposite poles of DHA in the pursuit of obtaining photo responsive liquid crystalline materials.

References


Liquid crystal dimers; A molecular level and mesoscale study

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Liquid crystal dimer molecules have shown a curious and as yet not fully characterised phase transition between the nematic and smectic phases via a new phase occupying a narrow window of temperature. We use a combination of simulation techniques in order to elucidate the local structure of this new phase.

The new phase is commonly attributed to two structures. One hypothesis, a pretransitional cybotactic nematic structure where small, uni-aligned smectic domains give rise to a biaxial signature. Alternatively, a twist-bend nematic has been proposed, where the local nematic director precesses about the global director helically, with minimal disruption to the nematic phase.

The uncertainty in the nature of this new nematic phase has lead researchers to name it the Nx phase. The thermodynamic range of stability is small, hence, experimental studies are limited in both the structural data they can provide and the degree of certainty. In contrast, structural characterisation is trivial from the output of a simulation.

To provide a molecular level picture we show two levels of simulation, i) a representation combining anisotropic Gay-Berne sites and Lennard-Jones particles, and ii) a soft, purely-repulsive DPD like model applied to systems sizes of up to $10^6$ molecules. The two models reproduce some of the key features of the molecular system and can provide further explanation as to the nature of the Nx phase.

Both models demonstrate a tendency to form smectic structures at least on the local level. However, where long range structure is accessible a more complex orientational and positional order is observed.

Figure 1: A schematic representation of the dimer molecule using Gay-Berne and Lennard-Jones particles (top). A snapshot from the simulation of this model in the smectic phase (bottom left) and a snapshot from a DPD simulation (bottom right).