18th International Conference on Ferroelectric Liquid Crystals
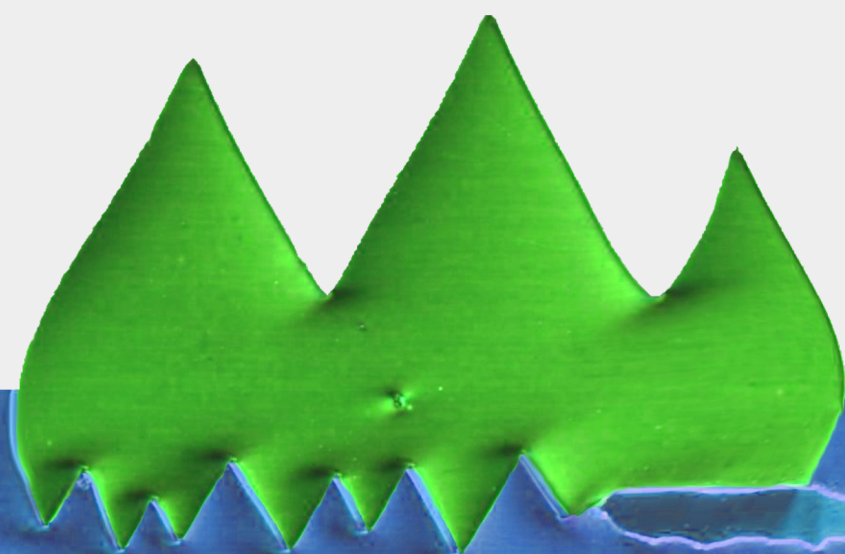
Polarity and Chirality in Soft Matter

September 6–10, 2021

Ljubljana, Slovenia

Book of Abstracts

Editor: Mojca Vilfan

Institut "Jožef Stefan"
Ljubljana, Slovenija

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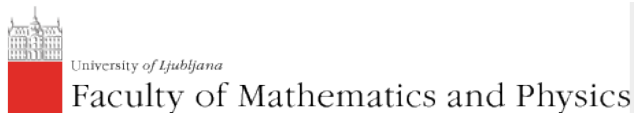# Polarity and Chirality in Soft Matter

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Editor: Mojca Vilfan,
J. Stefan Institute, Ljubljana, Slovenia and
Faculty of Mathematics and Physics, University of Ljubljana, Slovenia

Ljubljana, September 2021

Organised by: J. Stefan Institute, Ljubljana, Slovenia
and Faculty of Mathematics and Physics, University of Ljubljana, Slovenia

**Institut
"Jožef Stefan"
Ljubljana, Slovenija**

University of Ljubljana
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Monday, September 6

8:00	Registration
8:50	Opening ceremony
Chair	Alenka Mertelj
9:20	**PL1: Richard Mandle** An unexpected discovery of a new nematic phase
10:00	**O1: Mingjun Huang** How far can we push the length limit of rod mesogens for ferroelectric nematic liquid crystals?
10:20	Poster pitches: P1-P3
10:30	Coffee break
Chair	Alberta Ferrarini
11:00	**I1: Satoshi Aya** Topology and electro-optic properties of ferroelectric nematic materials
11:30	**O2: Nerea Sebastián** Investigations of the nematic to ferroelectric nematic transition
11:50	**O3: Peter Salamon** Droplets and inverse droplets of a polar nematic material in electric fields
12:10	Poster pitches: P4-P7
12:30	Lunch
Chair	Hajnalka Nadasi
14:00	**I2: Carsten Tschierske** Chirality synchronization in fluids by network formation
14:30	**O4: Matthias Lehmann** Design of polar subphthalocyanine star mesogens for photoconductive materials – alignment, photophysical and electronic properties
14:50	**O5: Alberto Concellón** Electric-field-induced chirality in columnar liquid crystals
15:10	Poster pitches: P8-P12
15:30	Coffee break
Chair	Alexey Eremin
16:00	**I3: Ivan Smalyukh** Pseudo-polar orientational order in monoclinic nematics
16:30	**O6: Gregory Smith** Existence of the B-Form DNA helix in nanoDNA liquid crystals and its variation due to aggregate assembly
16:50	Poster pitches: P13-P16
17:20	On-site poster session
19:00	End of day 1

An Unexpected Discovery of a New Nematic Phase

Richard J. Mandle[1,2*], John W. Goodby[2], Nerea Sebastian[3], Alenka Mertelj[3]

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[3]Jožef Stefan Institute, Jamova 39, SI-1000 Ljubljana, Slovenia

Uniaxial nematic phases are ubiquitous in our daily lives thanks to their use in display technology, and so the discovery of new nematic phase types generates great excitement. In the early 20th century, Born and Debye noted the possibility of a polar and ferroelectric nematic, a phase that has obvious applications potential.

In November 2009 I synthesised *RM230* (fig 1a); an unremarkable looking molecule decorated with a lateral methoxy unit for the purpose of reducing the melting point. *RM230* was found, unexpectedly, to exhibit two nematic phases. [1] *RM230* displays multiple diffuse low-angle X-ray scattering peaks (fig 1e), while optical textures display periodic structures (fig 1c). After an arduous journey to publication, [2] and the synthesis of many derivatives such as *RM734* (fig 1a), [3] the lower temperature nematic phase exhibited by these materials was shown to be a splay-modulated nematic phase, [4] with polar order [5] and ferroelectric properties. [6] The seemingly prerequisite combination of large molecular electric dipole moment and minimal aliphatic content endows materials such as *RM734* with high melting points; however, we have recently designed systems that display the Ns phase at ambient temperatures. [7]

In this talk, I will discuss the genesis of these materials, the role of molecular structure in the origin of this new nematic phase type, and the outlook for developing application-ready materials aided by computer simulations.

Fig. 1: (a) RM230/RM734; (b) POM of N (RM230, 94.4°C); (c) POM of N_S (RM230, 76.4°C); (d) N_S director map; (e) 2D SAXS of Ns (RM230, 72 °C)

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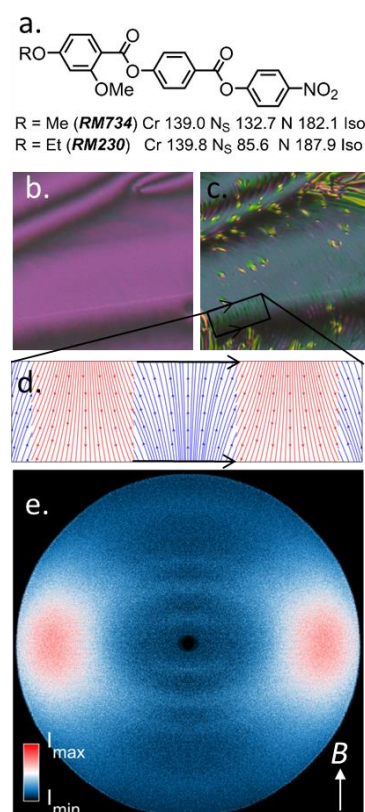
How far can we push the length limit of rod mesogens for ferroelectric nematic liquid crystals?

Jinxing Li[1], Satoshi Aya[1], Mingjun Huang[1]

[1] South China Advanced Institute for Soft Matter Science and Technology (AISMST), School of Molecular Science and Engineering, South China University of Technology, Guangzhou 510640, China.

Ferroelectric nematic liquid crystal (N_F) is a type of polar soft matter that was first discovered in 2017[1, 2]. It has an ultra-high dielectric constant (10^3-10^4 @ 1-10kHz) comparable to perovskite-based ferroelectrics. The strong nonlinear optical signal, combined with the unique fluidity of liquid crystal and response sensitivity to electric field[3, 4] makes N_F materials quite promising for the development of advanced liquid crystal optical or electrical devices. In our previous work[5], we systematically explored the transition pathway of the N_F phase in small liquid crystal molecules, as well as the topological structure and general molecular design strategy for the N_F phase. We have revealed the general molecular characteristics of N_F phase formation: the rod-shaped liquid crystal mesogen with dipole moment (μ) reaching 9 Debye (D), and the direction of the overall dipole moment deviating from the molecular principal axis by a certain angle (10°-30°). However, all the studied rod-shaped liquid crystal molecules have limited length range, around 2 nm. In this work, we increase the size of the rod-shaped aromatic oligomer mesogens (polymerization degree n = 1-12) and dipole moment value (6-30 D) through precise step synthesis (Figure 1), so as to continuously improve the dipole-dipole interaction among rod mesogens, which plays as the driving force for N_F formation. The widespread existence of N_F liquid crystal phase is far beyond our expectations, and thermodynamically stable N_F liquid crystal phases can be observed in all the oligomers with n ranging from 1 to 12 (with length larger than 7 nm). This work could largely deepen our understanding of N_F liquid crystal phase.
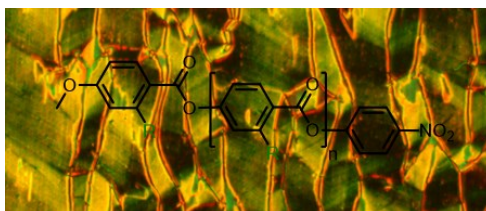

Figure 1: Precise oligomer liquid crystal mesogens

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Topology and electro-optic properties of ferroelectric nematic materials

Satoshi Aya[1,2], Junichi Kougo[1,2], Junchen Zhou[1], Xiuhu Zhao[1], Yuki Hisai[3],
Hiroya Nishikawa[4], Jinxing Li[1], Shuqi Dai[1] and Mingjun Huang[1,2]

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[2] *Guangdong Provincial Key Laboratory of Functional and Intelligent Hybrid Materials and Devices, South China University of Technology, Guangzhou 510640, China*
[3] *Money Forward, Inc. Shibaura, Minato-ku, Tokyo, Japan*
[4] *Physicochemical Soft Matter Research Team, RIKEN Center for Emergent Matter Science (CEMS), Japan*

Magnetic and electric states are closely related. However, many fundamental magnetic states cannot find their electric counterparts especially in liquid matter systems. Typically, many complex electromagnetic states require low symmetries of matters. Thereby, their appearance is limited mostly in solid-state materials, hindering the material processibility and tunability for a wide range of applications.

Recently, there emerged a new class of materials, dubbed splay nematic or ferroelectric nematic, where the head-to-tail symmetry of the traditional nematic state is broken. Here, we report on several novel electric analogues to the magnetic states, including the ferroelectric and new helielectric nematic states. All the matter states exhibit polar ordering in addition to the traditional local nematic orientational ordering. The systematic studies are composed of (1) machine-learning-guided massive synthesis from the fluidic monomer to moldable polymer materials, (2) structure and topological characterizations, and (3) determination of both the dielectric and nonlinear optic coefficients. On the conference, we will discuss the detailed topology and electro-optic properties of the matter states.
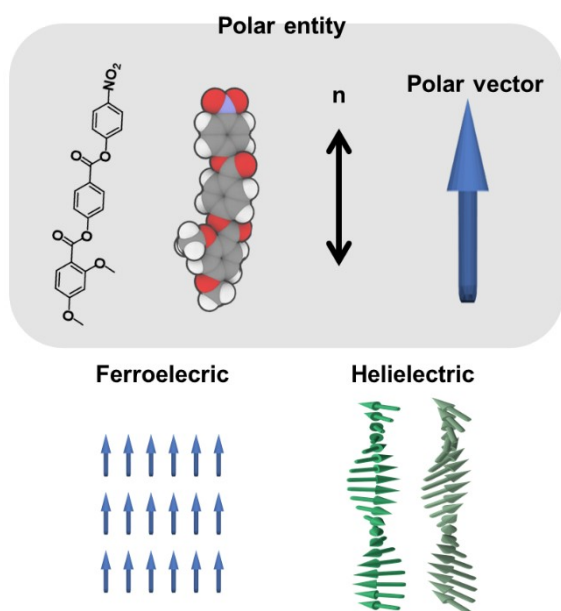
Figure 1: Ferroelectric and helielectric nematic Structures formed by polar entities. As an example, The polar entity of RM734 is shown.

Investigations of the nematic to ferroelectric nematic transition

Nerea Sebastián[1], Richard J. Mandle[2], Andrej Petelin[1,3], Irena Drevenšek Olenik,[1,3] Alexey Eremin[4], Martin Čopič[1,3] Alenka Mertelj[1]

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[2] School of Physics and Astronomy, University of Leeds, Leeds, UK
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The recent discovery of the ferroelectric nematic phase [1-3] certainly constitutes an important milestone in liquid crystals research. With it experimental investigation of one of the most searched liquid crystal phases in decades has finally been made possible, with high expectations for future applications. The first examples of materials showing the NF phase, RM734 [2,4,5] and DIO [3], have led to a number of new materials made of elongated molecules with large dipole moments exhibiting stable N_S phase [6] in the past two years, broadening the investigation possibilities. Here, we will give an overview of our investigations on RM734, with special focus on the behaviour at the nematic to ferroelectric nematic transition. We will show the optical textures at the transition and compare them with SHG microscopy images [7]. We will analyse the viscoelastic properties studied by c-DDM and DLS methods, showing strong softening of splay fluctuations in the N-N_S transition. We will correlate such observations with the observed softening of the collective dielectric relaxation mode [4].
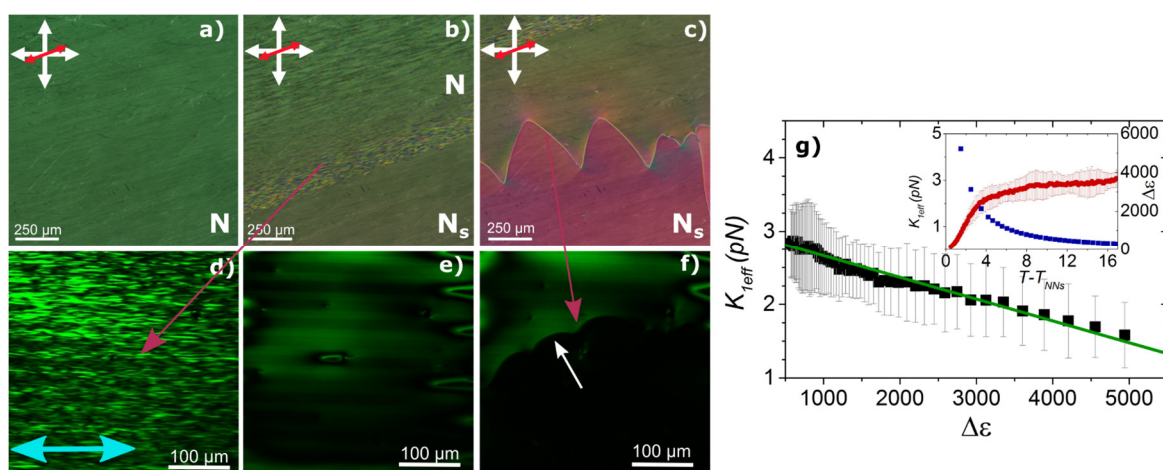

Figure 1: (a-b) POM snapshots across the N–N_S transition. Crossed arrows indicate the direction of polarizer and red arrow the cell´s rubbing direction. (d-f) SHG snapshots across the the N–N_S transition. Blue arrow shows direction of incoming polarization (along the rubbing direction). (g) Measured values of $K_{1,eff}$ vs interpolated values of $\Delta\varepsilon_{\parallel,1}$. Inset shows the temperature dependence of both K_1 and $\Delta\varepsilon_{\parallel,1}$ a few degrees above the transition to the Ns phase.

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Droplets and inverse droplets of a polar nematic material in electric fields

Marcell Tibor Máthé[1,2], Chenrun Feng[3], Rony Saha[3], Antal Jákli[1,3], and
Péter Salamon[1]

[1] *Wigner Research Centre for Physics, Budapest, Hungary*
[2] *Eötvös Loránd University, Budapest, Hungary*
[3] *Advanced Materials and Liquid Crystal Institute, Kent State University, Kent, OH 44242, USA*

The existence of a polar nematic phase was confirmed experimentally recently [1-3]. The novel phase with reduced symmetry exhibits huge spontaneous polarization, and therefore exceptional sensitivity to electric fields, which makes its discovery important not only from a scientific point of view, but an emergence of new class of liquid crystals promises high potential in applications as well. Previous studies focussed on investigating the properties of the polar nematic material confined between two flat walls. In order to achieve deeper understanding of the structure of the polar nematic phase, its interaction with electric field and the effect of confinement with non-flat walls, we performed our experimental investigations in two geometries with curved boundaries, using the compound RM734. The first geometry is well described by a spherical cap, which was realized in sessile droplets. The second case included air bubbles (gas inclusions) in the liquid crystal. We exposed the liquid crystal to electric fields with different directions, frequency, amplitude and time symmetry. We will present what kind of structures are realized (see some examples in Figure 1) in the studied geometries and how electric field can affect them. Specifically, we will discuss the shape change of the bubbles as a function of electric field.
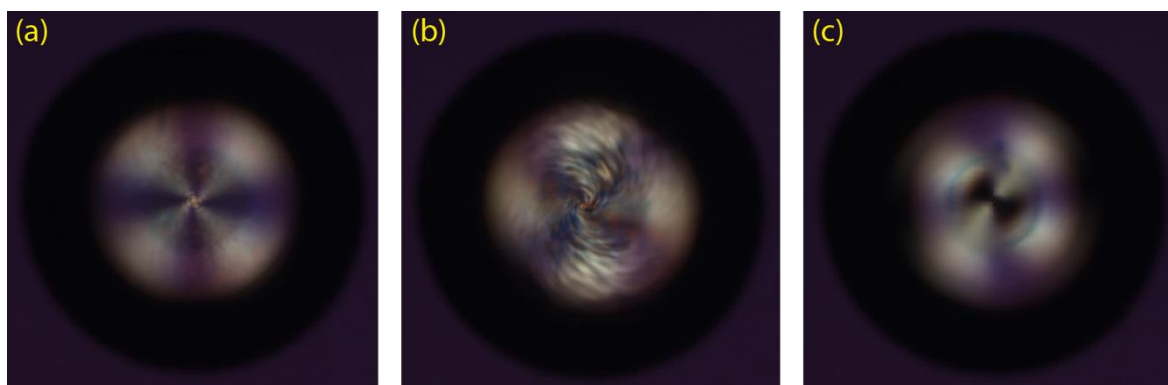

Figure 1: Texture of an RM734 droplet in the normal nematic phase (a), close to the transition to the polar phase (b), and in the polar nematic phase (c).

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Chirality Synchronization in Fluids by Network Formation

Carsten Tschierske[1], Christian Dressel[1], Tino Reppe[1], Mohamed Alaasar[1], Ohjin Kwon[1], Xiangbing Zeng[2], Goran Ungar[2], Feng Liu[3]

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[3] *Xi'an Jiaotong University, Xi'an, P. R. China.*

Since the discovery of the helical nanofilament and dark conglomerate phases in bent-core liquid crystalline systems spontaneous mirror symmetry breaking in LC systems has received significant attention. A newly emerging class of compounds, forming spontaneously mirror symmetry broken liquids and liquid crystalline phases is provided by polycatenar molecules showing conglomerate formation in their bicontinuous cubic phases [1-3] as well as in the adjacent liquid phases.[2,4]

In this talk the progress in this field is summarized and the present understanding of the underlying mechanism of mirror symmetry breaking, their relations to the molecular structure, as well as their wider implications will be discussed. Attention will also be focussed on diastereomeric relations between the transient supramolecular and the fixed internal (molecular) chirality, and the chirality amplification with external chirality sources. Figure 1 shows the fundamental chemical structures of the discussed molecules.
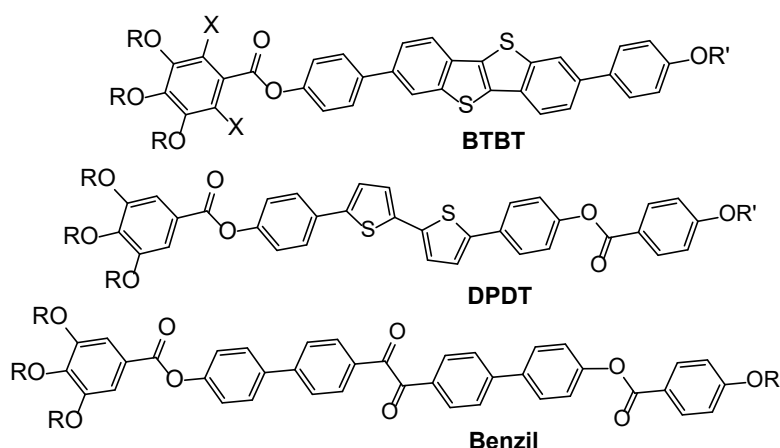

Figure 1: Chemical structures of the polycatenar mesogens under discussion.

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Design of polar subphthalocyanine star mesogens for photoconductive materials – alignment, photophysical and electronic properties

Matthias Lehmann[1,2], Maximilian Baumann[1], and Alexey Eremin[3]

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[3] Institute of Physics, University of Magdeburg, 39106 Magdeburg, Germany

The combination of anisotropy and fluidity in liquid crystals allows to manipulate anisotropic properties by external stimuli. For photoconductive applications, organic materials can be tailored to optimize absorption and to fit energy levels for charge separation, but it is an enormous challenge to combine the other prerequisites – the nanostructure of a p-n junction, and alignment of the structure between the electrodes [1]. The recent discovery of photo current in polar subphthalocyanines offers new promising perspectives to solve these problems [2]. The polar structure may facilitate charge separation and promotes the correct homeotropic alignment of the materials in an electrical field. Here, we present the design and synthesis of umbrella-shaped polar star mesogens with a subphthalocyanine core and oligo(thienyl) arms. While the shortest arm derivative self-assemble in a conventional columnar phase with a single mesogen as a repeat unit, the larger derivatives generate dimers that pile up into liquid crystal columns. Parallel dimers in polar columnar LC phases are confirmed by X-ray scattering, experimental densities, dielectric spectroscopy, second harmonic generation, alignment and conductivity studies. UV-Vis and fluorescence spectroscopies reveal a broad absorption in the visible range and only weak emission of the Q-band. Thus, these light-collecting molecules forming strongly polar columnar mesophases are attractive for application in the area of photoconductive materials.
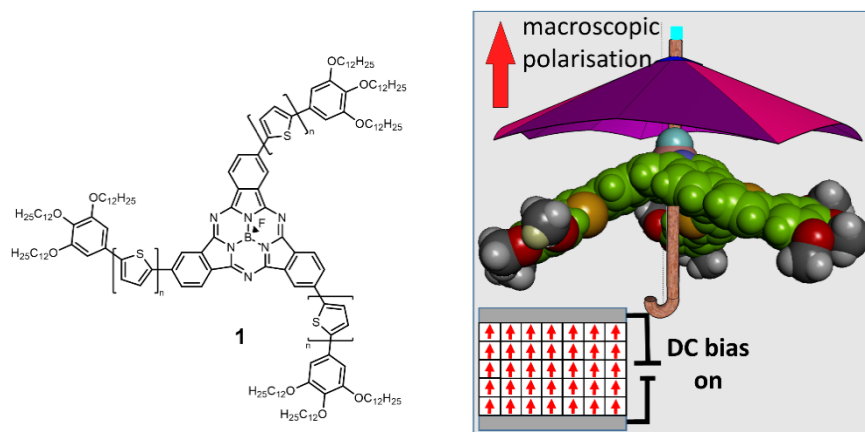
Figure 1: Conference webpage banner

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Electric-Field-Induced Chirality in Columnar Liquid Crystals

Alberto Concellón, Ru-Qiang Lu, Kosuke Yoshinaga, Hsiu-Fu Hsu, and
Timothy M. Swager

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Liquid crystals (LCs) are one of the most appealing synthetic helical systems due to the unique combination of long-range order and fluidity with chirality.[1] Among chiral LCs, columnar phases represent a powerful tool to achieve helical columnar assemblies that have demonstrated unusual electro-optical behavior, chiro-optical properties, ferroelectricity, or exceptional second-order non-linear optical susceptibilities.[2]

In this work, we describe a novel class of tetraphenylbenzene-based discotic molecules with exceptional self-assembling properties. Absorption and fluorescence studies confirmed the formation of *J*-type aggregates in solution. The discotic mesogens also show an enhancement of the emission upon aggregation. Interestingly, these discotic molecules displayed enantiotropic hexagonal columnar liquid crystal phases that can be switched into a helical columnar organization by application of an electric field. The helical columns arise from the electric-field-induced tilt of the polar fluorobenzene ring that directs all of peripheral phenyl groups into a propeller-like conformation with respect to the central benzene core. A cooperative assembly process of these propeller-shaped molecules resolves into a helical columnar organization, in which the preferred helical sense is obtained from the stereogenic center proximate to the polar carbon-fluorine bond. The ease of inducing chirality in columnar LCs by electric field presents opportunities to create next-generation chiral materials for a variety of applications, such as chiro-optical switches or chiro-magnetic materials.
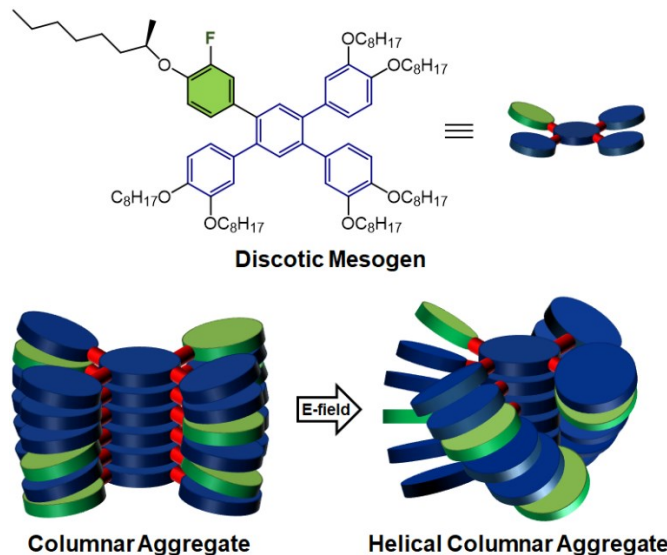
Discotic Mesogen

Columnar Aggregate → E-field → **Helical Columnar Aggregate**

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# Pseudo-polar orientational order in monoclinic nematics

Ivan I. Smalyukh[1,2,3]

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[3]*Renewable and Sustainable Energy Institute, National Renewable Energy Laboratory and University of Colorado, Boulder, CO 80309, USA*

Deep relations are believed to exist between symmetries of building blocks and condensed matter phases they form. However, to have a structure with few or no symmetry operations apart from trivial has so far been demonstrated to be a property of solids alone, but not of their fully fluid condensed matter counterparts. This lecture will discuss how dispersing highly anisotropic charged colloidal discs in a nematic host composed of molecular rods provides a platform for observing many low-symmetry liquid crystalline phases [1]. Depending on temperature, concentration and surface charge of the discs, we find nematic, smectic and columnar organisations with symmetries ranging from uniaxial to orthorhombic and to monoclinic. With increasing temperature, we observe unusual transitions from less to more ordered states and even re-entrant phases. Most importantly, we demonstrate the presence of monoclinic colloidal nematic order as well as the possibility of thermal and magnetic control of low-symmetry self-assembly [1]. We characterize this pseudo-polar monoclinic orientational order, along with the phase diagrams, orientational distribution functions and order parameters. Our experimental findings are supported by theoretical modelling of the colloidal interactions between discs in the nematic host and may provide a route towards realising myriads of new condensed matter phases in systems with dissimilar shapes and sizes of building blocks, as well as their technological applications.
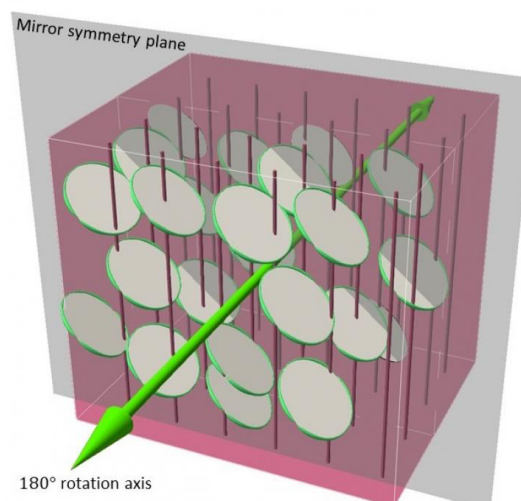
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Existence of the B-Form DNA helix in nanoDNA liquid crystals and its variation due to aggregate assembly

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[2]ESPCI Paris, Institut Pierre-Gilles de Gennes, Paris, France
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We show using diffraction of a synchrotron X-ray microbeam that liquid crystalline aggregates of 12mer nanoDNA, such as the Drew-Dickerson Dodecamer (DD), demonstrate a marked B-form DNA double-helix with only marginally less order than seen in longer DNA, such as the calf-thymus DNA used by Rosalind Franklin to produce the historic Photo 51 (Figure 1). This finding is significant because it shows that B-form helical order persists in liquid crystals of DD even though the backbone of the column contains a double-strand break at every twelfth position and the DD segments are not held rigidly in place as part of a crystal. The coherence of the B-form helix is influenced by the mode of aggregate self-assembly, where aggregates assembled by a base-paired sticky-end produce much longer helical correlation lengths than those formed by hydrophobic blunt-ends. Finally, we found that aggregates of blunt-end 4mer oligomers shorter than half of a single B-form helical turn no longer display the B-form helical diffraction pattern but order with a different structure. This study gives fundamental insight into the extent to which the classical DNA helix is affected by discontinuity in the polymer backbone.
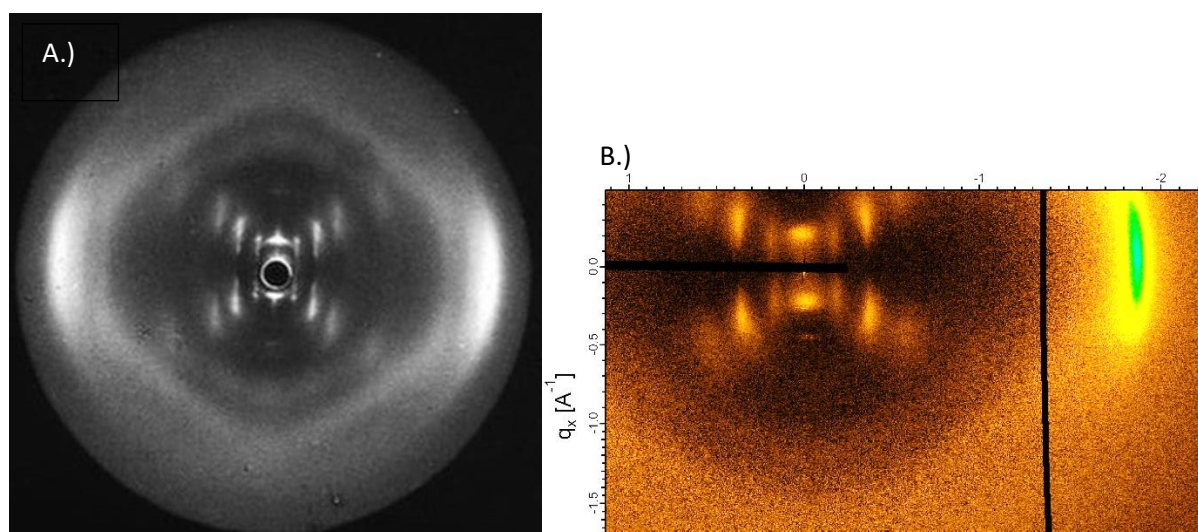

Figure 1: DNA X-ray diffraction A.) Photo 51, rotated and color inverted [1] B.) Columnar phase of DD nanoDNA as illuminated by X-ray microbeam.

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Tuesday, September 7

Chair	Kristiaan Neyts
9:00	**I4: Jan Lagerwall** Enabling technological revolutions with the endless potential of Cholesteric Spherical Reflectors (CSRs)
9:30	**O7: Inge Nys** Surface induced metastable chiral liquid crystal structures with hysteresis switching
9:50	**O8: Natalia Podoliak** Smectic A layers undulations manifested through the stripe textures in achiral liquid crystals
10:10	Poster pitches: P17-19
10:30	Coffee break
Chair	Slobodan Žumer
11:00	**I5: Oleg Lavrentovich** Optics and material properties of oblique helicoidal cholesterics
11:30	**O9: Migle Stebryte** Forward diffraction by chiral liquid crystal gratings with inclined helical axis
11:50	**O10: Wojciech Tomczyk** Flexopolarization and its role in the formation of twist-bend nematic phase: bridging theory and experiment
12:10	Poster pitches: P20-P22
12:30	Lunch
Chair	Peter Salamon
14:00	**I6: Antal Jákli** Multiple ferroelectric nematic phases of a highly polar liquid crystal compound
14:30	**O11: Žiga Gregorin** Dynamics of domain formation in a ferromagnetic liquid
14:50	Poster pitches: P23-P28
15:20	Coffee break
Chair	Martin Čopič
16:00	**O12: Joseph Maclennan** Experimental studies of the structure and phase behaviour of two ferroelectric nematic liquid crystals
16:20	**PL2: Noel Clark** Antiferroelectric Smectic Ordering as a Prelude to the Ferroelectric Nematic: Introducing the Smectic Z Phase
17:20	Online poster session (Gather.town)
19:00	End of day 2

Enabling technological revolutions with the endless potential of Cholesteric Spherical Reflectors (CSRs)

Yong Geng, Rijeesh Kizhakidathazhath, Hakam Agha, and Jan P.F. Lagerwall

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The seemingly simple step of molding a cholesteric liquid crystal into spherical shape with radial helix can have profound consequences. In my talk I will show how the omnidirectional selective retroeflectivity of such Cholesteric Spherical Reflectors (CSRs) gives rise not only to intriguing optical phenomena [1–2] (a-b), but also to an astounding number of application opportunities with revolutionary potential. After having demonstrated that CSR arrays are Physical Unclonable Functions (PUFs) [2], of great interest for anti-counterfeiting and supply chain traceability [3], we are now developing a human-invisible infrastructure to support self-driving cars and other autonomous robots in human-populated environments [3–4]. Polymerized CSRs (c) tuned to near-UV or IR reflection are organized into 'fiducial markers' (similar to QR codes) placed on any objects with which a robot needs to interact. The markers link the objects to their 'digital twins' in a computer model of the environment. Key to these possibilities is the circular polarization of the reflection, which allows extremely efficient background subtraction (d–g). We are also developing the concept for life vests, to assist in search-and-rescue operations at sea, and in our most recent project we propose to boost the detection limit of Rapid Antigen Tests for diseases like COVID-19. By replacing the gold nanoparticles or died latex beads, currently used in standard Lateral Flow-based tests, by CSRs, we expect the contrast and thus the signal-to-noise ratio to be greatly improved.
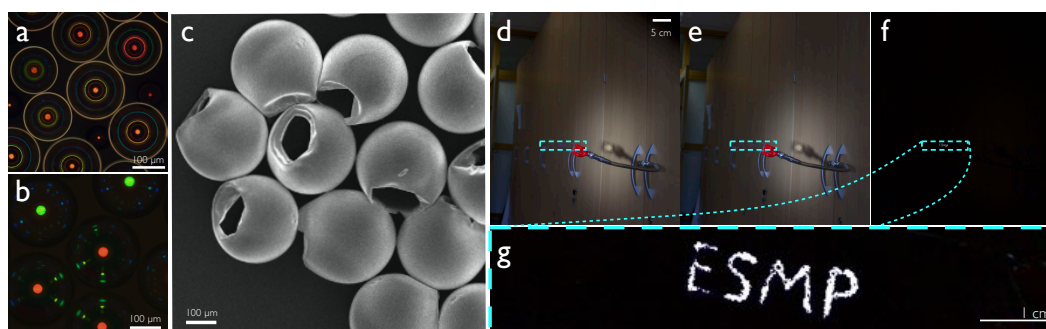

Figure 1: Polarizing microscopy images of CSR shells showing internal ring reflection (a) and cross communication (b). Electron microscopy image of polymerized CSRs (c). Demonstration of CSR-enabled information encoded into surfaces, with subtraction of an image through left-handed circular polarizer (e) from one through right-handed circular polarizer (d), leading to highly efficient background subtraction (f). The enlarged decoded message is shown in (g). From [4].

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Surface induced metastable chiral liquid crystal structures with hysteresis switching

Inge Nys[1], Brecht Berteloot[1], Jeroen Beeckman[1], and Kristiaan Neyts[1]

[1] Liquid Crystals and Photonics Group, Department of Electronics and Information Systems, Ghent University, Ghent, Belgium

The self-organization of liquid crystals (LCs) into stimuli-responsive hierarchical superstructures makes them interesting for integration in tunable electro-optic devices such as diffraction gratings, smart windows and lasers. To steer the LC self-organization, patterned surface anchoring can be applied, for example with the help of photo-alignment techniques. An almost arbitrary control over the surface anchoring is possible and the combination with chiral liquid crystal (CLC) provides additional freedom to design functional optical components. CLC, that spontaneously assembles into a helical structure, is known to give rise to metastable solitonic entities in strongly confined geometries. We demonstrate that metastable chiral structures can also be created with the help of patterned surface alignment. In this work the alignment direction on the bottom substrate varies periodically in the x-direction and on the top substrate it varies in the y-direction (figure 1). The combination with CLC leads to the formation of two different topological states at high and low voltages. Switching between both occurs via a hysteresis loop and the resulting optical properties can be steered by adjusting the surface alignment period, the cell thickness and the amount of chirality in the LC.

Figure 1: schematic illustration of the surface alignment pattern (left) and polarizing optical microscopy images for low and high applied voltages (right).
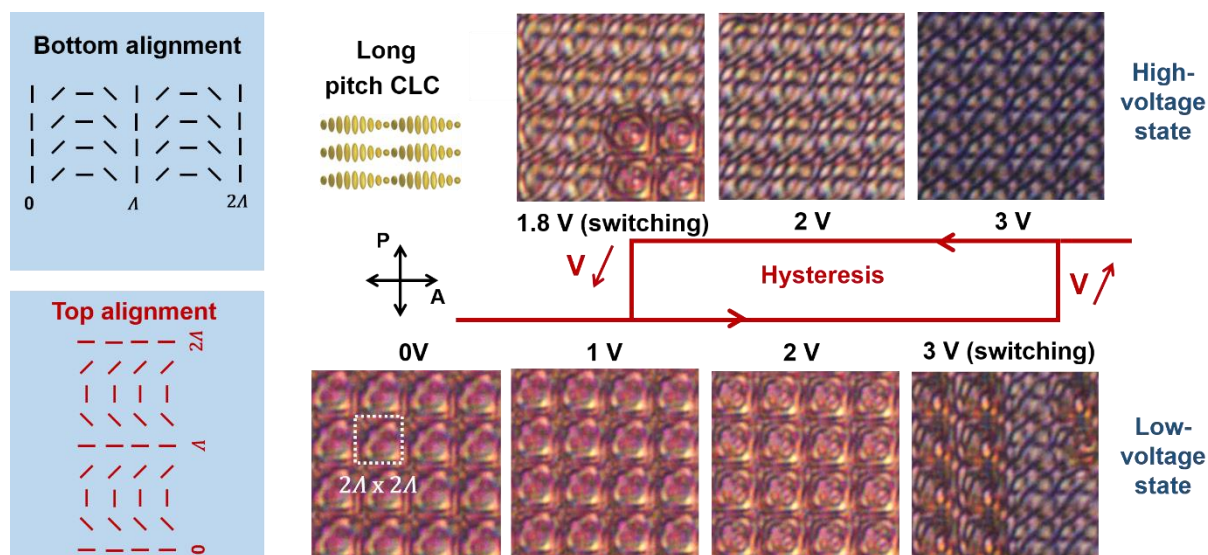
Apart from the experiments also finite element Q-tensor simulations are performed to reveal the 3D director configuration. We focus on the topology of the novel CLC structures, the effect of chirality, the deformation under application of an electric voltage and the hysteresis when switching from one state to another. These results are of fundamental interest and open up applications for ultra-low power devices such as diffraction gratings with internal memory. This may find applications in smart windows that can operate several optical states without consuming power.

Smectic A layers undulations manifested through the stripe textures in achiral liquid crystals

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Stripe textures in layered systems represent regular variations of optical axis due to the structural modulations, which can appear as a result of different external stimuli: strain [1], electric field in electroclinic materials [2], layer contraction at the SmA-SmC phase transition [3]. Herein we report on the experimental evidence of a regular stripe pattern in the liquid crystalline smectic A (SmA) phase for achiral compounds in the bookshelf geometry, which has not been reported without an external influence so far.

Under a polarising microscope (POM) we observed the stripe pattern in the SmA phase upon heating for several non-chiral compounds. We studied the stripes' parameters for various cells thicknesses and we found that for thin 1.7µm cells a simple periodic structure was present (Figure 1a). For thicker cells more complex periodic structures have been observed (Figure 1b). Due to the spatial variation of the optical axis, the samples acted as diffraction gratings. Based on a detailed analysis, we obtained parameters of the modulated structure from the diffraction experiments of polarised light (Figure 1c). The period and the character of the undulations depended on the sample thickness and was in micrometre region; the amplitude of the undulations was in the order of tens of nanometres. Additionally, we probed the samples by imaging polarimetric experiments and the obtained modulation parameters corresponded well with the results obtained from POM and diffraction.

Our observations were explained by the undulations of the smectic layers, which appeared as a result of the strain acting on the layers due to their contraction during heating because studied materials possess high negative values of the thermal expansion coefficient. We proposed a theoretical model based on the free energy density to describe the observed behaviour.
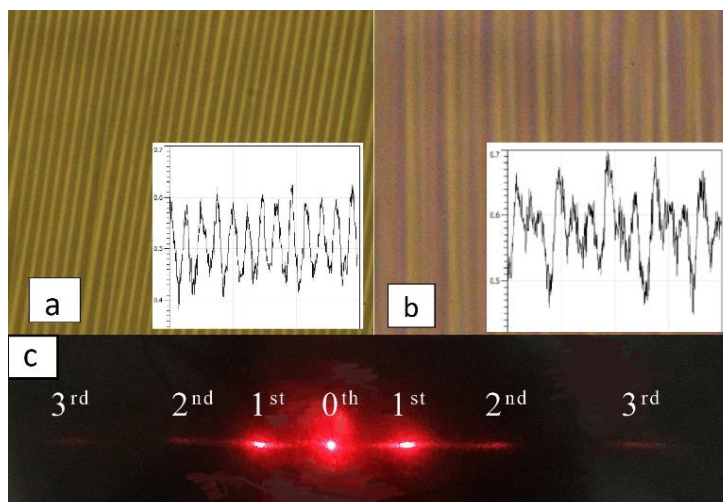

Figure 1: a) striped texture for thin 1.7 µm cell; b) texture of the more complex periodic structure for 5 µm cell; c) diffraction pattern for thin 1.7 µm cell. In the insets of Figures 1a) and 1b) the intensity profiles perpendicular to the stripes are presented.

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Optics and material properties of oblique helicoidal cholesterics

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An attractive feature of cholesterics for optical applications is that the pitch and thus the wavelength of diffraction respond to temperature or chemical composition changes. However, the most desired mode of pitch control, by electromagnetic fields, has so far been elusive. Synthesis of bent-shape flexible dimer molecules resulted in an experimental realization of a new cholesteric state with an oblique helicoidal structure, abbreviated as Ch_{OH} [1]. The Ch_{OH} state forms when the material is acted upon by the field and aligns its axis parallel to the field. The principal advantage of Ch_{OH} is that the field changes the pitch but preserves the single-harmonic heliconical structure. As a result, the material shows an extraordinarily broad range of electrically tunable robust selective reflection of light, from ultraviolet to visible and infrared. The Ch_{OH} also responds to the photoinduced molecular transformations. We demonstrate how the Ch_{OH} response could be used to measure material properties of chiral liquid crystals such as elastic moduli [2] and a combined electric field-light irradiation control of Bragg reflection at the Ch_{OH} structure.

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Forward diffraction by chiral liquid crystal gratings with inclined helical axis

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Liquid Crystals and Photonics group, ELIS department, Ghent University, Ghent, Belgium

This work is focused on the reflective diffraction gratings based on chiral liquid crystals – optical components with a high diffraction efficiency and unique polarization selectivity. It has been shown that if the liquid crystal has a periodically rotating anchoring pattern at the substrates, the liquid crystal in the bulk self-organizes into a structure such that the liquid crystal planes with a constant director orientation are inclined with respect to the substrate plane. The two competing theories for the director configuration in the bulk have been proposed in literature. One of them suggested that the director is parallel to the substrate [1] while the other one claimed that the director is parallel to the tilted planes of constant director [2]. In our previous work we reported that the polar angle of the molecules is not constant and varies along the thickness of the layer [3]. We now provide analytical formulae for azimuthal and polar angles of such a structure [4] and prove that this theoretical model is correct by comparing experimental measurements of transmission spectra with numerical simulations of such reflective diffraction grating structure (see Figure 1). In order to further investigate the behaviour of such device we also compare the spectral behaviour to the one of the planar chiral liquid crystal layer. In this work several new phenomena were discovered and explained: appearance of a full-reflection band at large angles of incidence, forward diffraction with a lateral shift and the influence of the different layers in the structure on the optical properties.
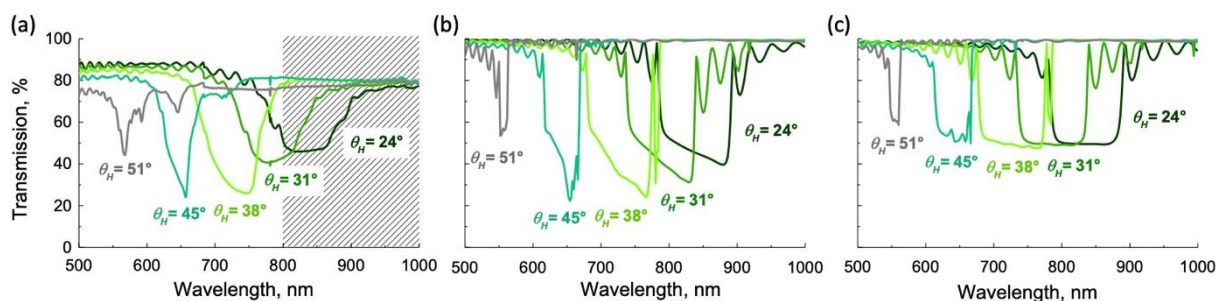

Figure 1: (a) Measured transmission spectra of CLC grating with a period of 700 nm for TE polarization for different angles with respect to the helical axis θ_H. Numerically calculated transmission spectra for TE polarization for different angles θ_H assuming inclined helix (b) and vertical helix (c) models.

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Flexopolarization and its role in the formation of twist-bend nematic phase: bridging theory and experiment

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The past decade was full of new discoveries in liquid crystal science [1–5]. Many novel phases were reported, among which is the twist-bend nematic (N_{TB}). The uniqueness of this phase finds its manifestation through the formation as a result of the spontaneous chiral symmetry breaking in a liquid crystalline system of achiral bent-shaped molecules. The corollary of this phenomenon is an emergence of heliconical (1D modulated) structure of nanoscale pitch with a ground-state exhibiting a degenerate sign of chirality (ambidextrous chirality). In no time, N_{TB} attracted a worldwide interest, which pushed it to the forefront of hot topics in liquid crystal research [6].

We extended the minimal coupling Landau-de Gennes free energy expansion in terms of the symmetric and traceless tensor order parameter $Q_{\alpha\beta}(\mathbf{r})$ and its first-order derivatives $Q_{\alpha\beta,\gamma}(\mathbf{r})$ supplemented by the couplings with the polar field $P_{\alpha}(\mathbf{r})$ [7–9]. The main purpose of this study was to test whether the flexopolarization scenario, claimed to be responsible for observed chiral symmetry breaking, is capable of accounting quantitatively for experimental data known to date. The majority of constitutive parameters (i.a. elastic constants, flexopolarization coefficient, polar coupling) of the model are estimated from experimental data acquired for CB7CB compound in the nematic phase (N). Then we sought for relative stability and properties of the so-called homogeneously deformed structures (among which is the N_{TB} phase) with reference to the isotropic and nematic phases. Finally, we evaluated various properties of N_{TB} like temperature variation of the structure's wave vector, conical angle, polarization, and relevant order parameters. As it turns out, the extended theory accounts not only for qualitative but also quantitative features of N and N_{TB} and provides strong support for flexopolarization induced instability to be a legitimate mechanism for N-N_{TB} phase transition [10].

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Multiple ferroelectric nematic phases of a highly polar liquid crystal compound

Rony Saha[1,2], Pawan Nepal[3], Chenrun Feng[2,4], Md Sakhawat Hossein[4], James T. Gleeson[1], Samuel Sprunt[1,2], Robert J. Twieg[3], <u>Antal Jákli</u>[1,2,4]

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[2]*Advanced Materials and Liquid Crystal Institute, Kent State University, Kent, OH 44242, USA*
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Ferroelectric nematic liquid crystals [1-4] represent not only interesting fundamental science, but they are also hold promise for storage capacitors with high power density or new information display technology having sub-millisecond switching. In this talk we describe the synthesis and measurements of the physical properties of a new highly polar ferroelectric nematic compound, 4-nitrophenyl 4-[(2,4-dimethoxylbenzoyl)oxy]-2-fluorobenzoate (RT11001), see Figure 1. The dipole moment of this material (along the long molecular axis) is calculated to exceed 11.5 Debye.
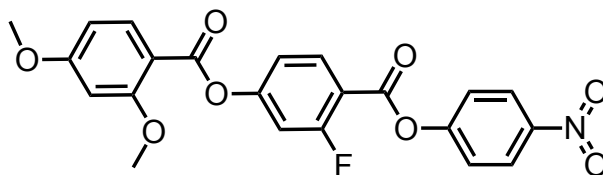
$$Iso - 161°C - N - 140.3°C - N_F - 112°C - F_2 - F_3 - 70°C - Cr$$

Figure 1: Molecular structure and phase sequence of RT11001

We will describe a wide range of physical characterization results including differential scanning calorimetry (DSC), mass density measurement, optical birefringence, polarizing optical microscopy (POM), electric current analysis, and electro-optical switching, to show that RT11001 has three distinct ferroelectric states, N_F, F_2 and F_3 with ferroelectric polarization reaching $P_o = 0.07 \frac{C}{m^2}$. N_F is a purely orientationally ordered ferroelectric nematic phase, F_2 has a ferroelectric nematic with possibly short-range hexagonal order normal to the director (N_{hF}), and F_3 probably has a long-range hexagonal order normal to the director (Col_{hF}).

We will also explain the benefits and disadvantages of using parallel plate and in-plane electrode geometries to study the electric properties of fluid ferroelectric liquid crystal materials.

The latest x-ray and other results of our ongoing research in this subject will be also discussed.

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Dynamics of domain formation in a ferromagnetic liquid

Žiga Gregorin[1], Patricija Hribar Boštjančič[1,3], Nerea Sebastián[1], Darja Lisjak[1], Natan Osterman[1,2], Alenka Mertelj[1]

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Traditional ferrofluids, suspensions of magnetic nanoparticles in an isotropic solvent, are indeed paramagnetic. First example of a ferrofluid with spontaneous ordering was achieved in suspensions of BaHF nanoplatelets in a nematic liquid crystal host [1,2]. Next the formation of ferromagnetic nematic phase in suspensions of platelet-based magnetic nanoparticles in an isotropic solvent was demonstrated. Spontaneous ferromagnetic nematic ordering is obtained above a certain threshold concentration [3], below which the suspension is isotropic but highly sensitive to magnetic fields. By varying the essential components of such ferrofluids, surfactant concentration, particle size distribution and magnetization, we were able to lower the threshold concentration, thus decreasing the material viscosity and its response times [4].

Ferromagnetic nematic suspensions form domain structures in which magnetic orientation of particles is well defined, analogous to the domain structure in solid state ferromagnets. However, the fluid-like character of the material makes the domain structure to be determined by confinement parameters e.g. the boundaries of the container and by the initial annealing field direction. The whole process of domain growth has to be done in a controlled environment with the magnetic field strength at least 50 times lower that Earth's magnetic field (also called zero field). It takes less than a second to see the shape of the domains like in Figure 1. With the material left in zero field for several hours interesting bend structures have also appeared in parts of the sample.
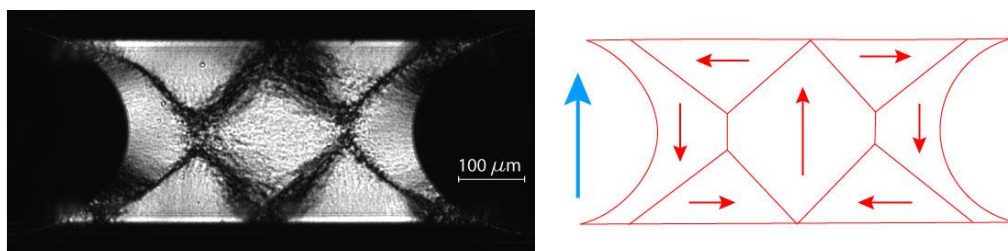

Figure 1: Polarizing optical microscopy image (left) and schematics (right) of domain structures with annealing magnetic field direction marked with blue and domain orientations in zero field marked with red.

On the other hand, isotropic suspensions are very sensitive to small magnetic fields and a field with strength as low as 1 µT results in field induced ordering. Additionally, phenomena such as flow induced ordering have also been studied.

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# Experimental studies of the structure and phase behaviour of two ferroelectric nematic liquid crystals

Xi Chen[1], Zhecong Zhu[1], Cheol Park[1], Eva Korblova[2], David M. Walba[2],
Matthew A. Glaser[1], Joseph E. MacLennan[1], Noel A. Clark[1]

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[2] Soft Materials Research Center, Chemistry Department, University of Colorado Boulder, USA

The Boulder group recently showed that the liquid crystal RM734 [1] possesses a ferroelectric nematic (N_F) phase [2]. In the search for additional ferroelectric nematics, we studied the liquid crystal DIO, which was previously reported to be "ferroelectric-like [3]. In an antiparallel-rubbed liquid crystal cell, polarized light microscopy of DIO in the polar phase reveals two twisted states of the director and polarization field that have opposite handedness. These chiral states can be converted from one to the other with an applied electric field. This phenomenology is similar to that observed in RM734 in the same type of cell. The ferroelectric polarization of DIO derived from the switching current generated during reversal of an in-plane field was found to be similar in magnitude to that of RM734. These observations confirm that the previously reported polar phase is indeed ferroelectric, as tentatively suggested by Nishikawa et al. [3].

We have also investigated the phase behaviour, miscibility, and electro-optics of binary mixtures of RM734 and DIO. As expected, the N_F temperature range in the mixtures is extended to lower temperatures, with field-induced molecular reorientation in response to a 10 V/mm, in-plane applied field observed at temperatures as low as 28°C in a 50:50 mixture. The temperature range of the M_2 phase between the N and N_F phases in DIO is reduced in the mixtures and disappears at higher RM734 concentration.
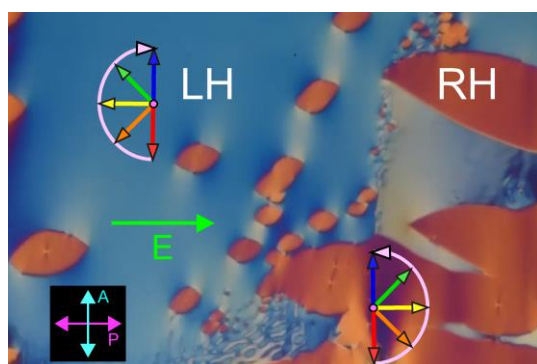
Left: π-twist domains of opposite handedness in DIO.
Right: Binary phase diagram of RM734 and DIO.
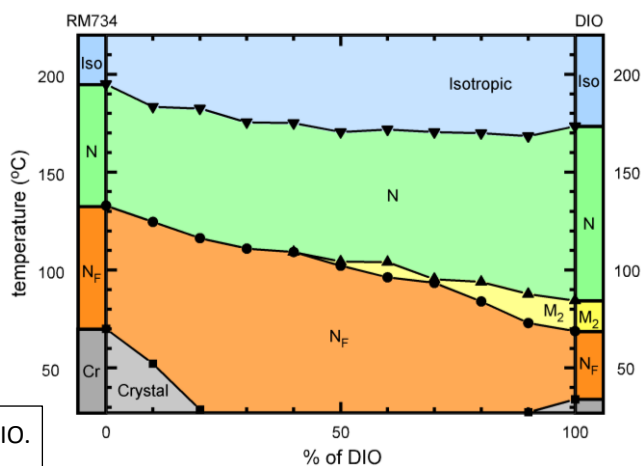
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Antiferroelectric Smectic Ordering as a Prelude to the Ferroelectric Nematic: Introducing the Smectic Z Phase

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Soft Materials Research Center, Department of Physics, University of Colorado, Boulder

The Boulder group* has studied the liquid crystal phase behavior of mixtures of RM734 and DIO over their full range of binary concentrations. These mixtures exhibit complete binary miscibility of the nematic (N), and ferroelectric nematic (N_F) phases. Extensive textural and electro-optic study shows their N_Fs are the same phase, a uniaxial, homogeneous, unmodulated ferroelectric nematic fluid, with, in absence of applied field, almost perfect polar ordering of rod-shaped, dipolar molecules. In RM734 a direct phase transition from the N to the N_F phase is observed, while, as previously reported [1], this transition takes place in DIO via an intermediate phase of unknown structure.

Here we report that this phase, between the N and N_F in DIO, is a new class of smectic liquid crystal, one having the molecular long axes on average *parallel* to the layers. Synchrotron-based non-resonant SAXS and electro-optical microscopy experiments show that the intermediate phase is density modulated with a 90Å periodicity. Figure 1 shows that its Bragg wavevector is normal to the magnetically aligned director, *n*, and thus that the layers are parallel to *n* (Fig.2). This geometry (tilt = 90º) is the limit opposite to that of the smectic A (tilt = 0º), so we call this phase the smectic Z. Upon cooling, the SmZ scattering peaks appear at $T \sim 83ºC$ as weak, diffuse spots, with integrated intensity that grows to maximum at $T \sim 76ºC$ and then decreases to zero at $T \sim 69ºC$, near the SmZ-N_F transition. The peak location, $q_M \sim 0.071Å^{-1}$, varies by only few percent over the SmZ range. The minimum peak width indicates a layering coherence length of over 1000Å. The N_F phase exhibits no diffraction to indicate modulation in this *SAXS* regime.
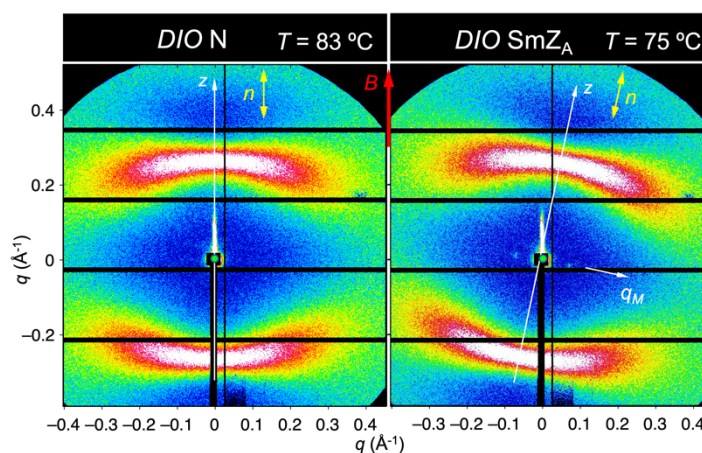

Figure 1: SAXS of magnetically-aligned DIO (field B) in the nematic (left) and SmZ phase (right). The horizontal white/red features are from head-to-tail molecular association. The SmZ diffraction spots are at $q_M = 0.071Å^{-1}$.

Figure 2: Bookshelf geometry of the SmZ_A phase in a cell with buffed planar alignment layers. In DIO the layers are ~ 90Å thick and antiferroelectric, giving an overall periodicity of 180Å.
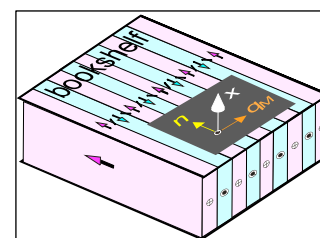
The space-filling periodic structure of the SmZ phase results in textures familiar in smectics, , such as the bookshelf layer organization in Fig. 2, including the formation of chevron textures having zig-zag walls, suppression of the Freedericksz deformation that rotates *n* out of the layer plane, and the stabilization of freely suspended smectic films. The SmZ is antiferroelectric, with polarization along *n* and oppositely directed in neighboring layers. The layer polarization density is small at the N-SmZ_A transition, increasing to near that of the N_F phase at lower temperatures. A reversible field-induced antiferroelectric to ferroelectric transition is observed, at a threshold field that decreases with *T*.

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

Wednesday, September 8

Chair	Nataša Vaupotič
9:00	**PL3: Ewa Górecka** Photonic band gap in achiral liquid crystals – a twist on a twist
9:40	**I7: Dong Ki Yoon** Light-driven fabrication of helical nanostructures for optical applications
10:10	**O13: Jun-ichi Fukuda** Simulation study of twin boundaries in cholesteric blue phase
10:30	Poster pitches: P29-P31
10:40	Coffee break
Chair	Miha Ravnik
11:10	**O14: Simon Čopar** Chiral topological states in flowing achiral nematics
11:30	**O15: Guilhem Poy** Optical solitons and chirality-enhanced nonlinear optical response in frustrated cholesterics
11:50	**O16: Liana Lucchetti** Pitch tuning induced by optical torque in heliconical cholesteric liquid crystals
12:10	Poster pitches: P32-P36
12:30	Lunch
14:00	End of day 3

Photonic band gap in achiral liquid crystals – a twist on a twist

D. Pociecha[1], N. Vaupotic[2,3], M. Majewska[1], E. Cruickshank[4], R. Walker[4], J. M. D. Storey[4], C. T. Imrie[4], C. Wang[5], <u>E. Gorecka</u>[1]

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For many decades it was generally believed that intrinsic molecular chirality was a prerequisite to drive the helical structure of a LC phase. If the wavelength of light fits the periodicity of the helix, then circularly polarized incident light with the same handedness as the helix is reflected – the photonic gap is formed. Recently, however, it has been shown that achiral mesogenic molecules may also form helical phases, allowing for fabricating photonic band gap structures from achiral materials. Unfortunately, the N_{TB} phase the helical pitch length is far from the optical range. The smectic analogues of the N_{TB} phase also exist, the SmC_{TB} phase might have a simple heliconical arrangement of molecules or more complex structure, with an additional longer helix of the order of tens of smectic layers superimposed on a short helix [1]. For the materials studied here, the transition between two types of the SmC_{TB} phase was found, at which the longer helix unwinds and its pitch becomes comparable to the optical wavelength. This leads to the well-known phenomenon of the selective reflection of light (Fig. 1) with an energy band gap in the visible range. This effect, although common for chiral liquid crystal phases, is reported here for the first time for achiral mesogens.
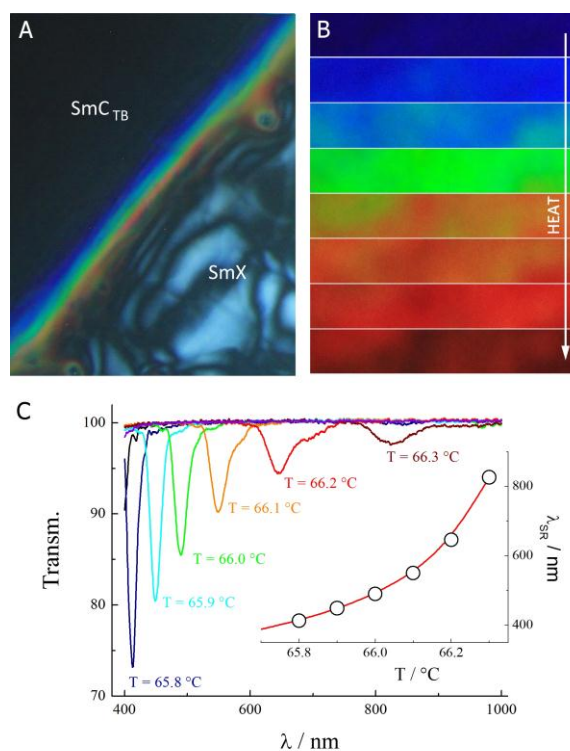

Figure 1. (A) Optical texture of CB6O.12 at the transition between two types of SmC_{TB} phase. The rainbow colours due to a selective reflection appear simultaneously because of a small temperature gradient in the sample. (B) A sequence of optical textures taken as a function of temperature (C) Transmission spectra as a function of temperature. The inset: position of the selective reflection band (λ_{SR}) vs. temperature.

[1] M. Salamończyk, N. Vaupotič, D. Pociecha, R. Walker, J. M. D. Storey, C. T. Imrie, C. Wang, C. Zhu, E. Gorecka, Multi-level chirality in liquid crystals formed by achiral molecules, *Nat. Commun.* **10**:1922, (2019).

Light-driven fabrication of helical nanostructures for optical applications

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Dong Ki Yoon[1,5]

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[5] Department of Chemistry and KINC, KAIST, Daejeon, Republic of Korea

Chiral liquid crystal phases show the fascinating structural and optical properties due to the inherent helical characteristics. Among various kinds of chiral LC phases, the helical nanofilament phase made of achiral bent-shaped molecules has been in keen interest due to the unusual polar and chiral properties [1]. This talk is intended to introduce the recent progress in the orientation control and its application of the HNF phase, which includes the photoalignment of the HNF phase, and chiroptical applications such as photonic crystal, chirality sensor, and security use. In detail, irradiating a film comprising azobenzene derivatives with UV light produces oriented arrays of HNFs via the photoisomerization-induced Weigert effect [2]. As a result, structural colors are observed due to the extrinsic chiral reflection in the visible wavelength range, and the reflected color can be tuned by adjusting the molecular length of the azobenzene derivative. We also have directly visualized optical activity of chiral samples using an orientation-controlled HNFs. Right- or left-handed domains of the HNFs are large enough to be seen with the naked eye, up to ~several mm^2 [3]. The periodic arrays of aligned HNFs reflect a specific color, here green, due to the Bragg reflection. Such a reflector enables an easy detection of optical activity of a sample placed on it. The device was tested with naturally chiral substances, like fructose and glucose, which exhibit opposite sense of optical activity, as well as with structurally chiral nematic LC phase and revealed high sensitivity of a detection. Indeed, we demonstrated security codes based on chiral photonic crystals made of HNFs that are not easy to be mimicked, which is quite different from the conventional technology used currently [4]. The HNF-based chiral photonic crystals show the structural colors changed depending on the polarization of the light in the transmission mode. These color changes are easily detected in real-time, which are useful to fabricate anti-counterfeiting patterns that show beautiful and diverse color changes during rotating polarizers. We believe these resultant optical applications can provide a new platform in various colors and further applications.
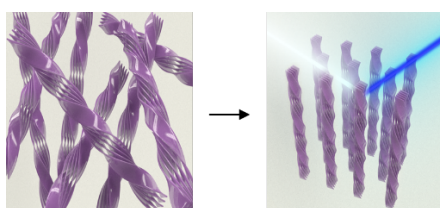

Figure 1: Orientation control of helical nanofilament

[1] Wongi Park, Dong Ki Yoon*, "Orientation Control of Helical Nanofilament Phase and Its Chiro-optical Applications", *Crystals*, 2020, **10**, 8, 675

[2] Wongi Park, Taewoo Ha, Teun-Teun Kim, Anna Zep, Hyungju Ahn, Tae Joo Shin, Kyung Ik Sim, Taek Sun Jung, Jae Hoon Kim, Damian Pociecha, Ewa Gorecka and Dong Ki Yoon* "Directed self-assembly of a helical nanofilament liquid crystal phase for use as structural color reflectors" *NPG Asia Mater*, 2019, **11**, 45

[3] Wongi Park, Damian Pociecha, Ewa Gorecka, Dong Ki Yoon*, "Direct Visualization of Optical Activity in Chiral Substances using a Helical Nanofilament (B4) Liquid Crystal Phase" *Advanced Optical Mater.*, 2019, 1901399

[4] Wongi Park, Taewoo Ha, Taek Sun Jung, Kyung Ik Sim, Jae Hoon Kim, Joanna M. Wolska, Damian Pociecha, Ewa Gorecka, Teun-Teun Kim* and Dong Ki Yoon*, "Security use of chiral photonic film made of helical liquid crystal structures" *Nanoscale*, 2020, **12**, 21629

Simulation study of twin boundaries in cholesteric blue phase

Akihiro Yamashita[1] and Jun-ichi Fukuda[1]

[1]*Department of Physics, Kyushu University, Fukuoka, Japan*

Cholesteric blue phases (BPs) are exotic three-dimensional ordered phases exhibited by highly chiral liquid crystals. They comprise a network of disclination lines and double-twist cylinders in which the orientational order is twisted along all directions perpendicular to the cylinder axis. Although the phase behavior of BPs has been extensively investigated, details of structural transformation between different BPs are still largely unknown. Recently, it was shown by X-ray scattering [1] that the transition from BP II to BP I can occur in a diffusionless manner like martensites, resulting in the coexistence of BP I lattices of different lattice orientations with twin boundaries. However, direct experimental observation of the real-space structures of twin boundaries is a challenge because of the characteristic length scale involved (a few hundred nanometer). Moreover, theoretical arguments on twin boundaries of atomic crystals cannot be simply applied, because BP lattices do not have discrete "lattice points." Here we investigate the structures of twin boundaries in BPs by numerical calculations based on the Landau-de Gennes continuum theory in which the orientational order is described by a second-rank tensor.

Figure 1 shows an example of structures obtained by minimizing the free energy functional. Disclination lines are bent but smoothly connected at the twin boundaries. Position of the BP I lattices with respect to the twin boundaries is also identified. We hope our study will motivate further theoretical studies on twin boundaries of soft materials with crystalline order, and also experimental studies towards their direct observation.
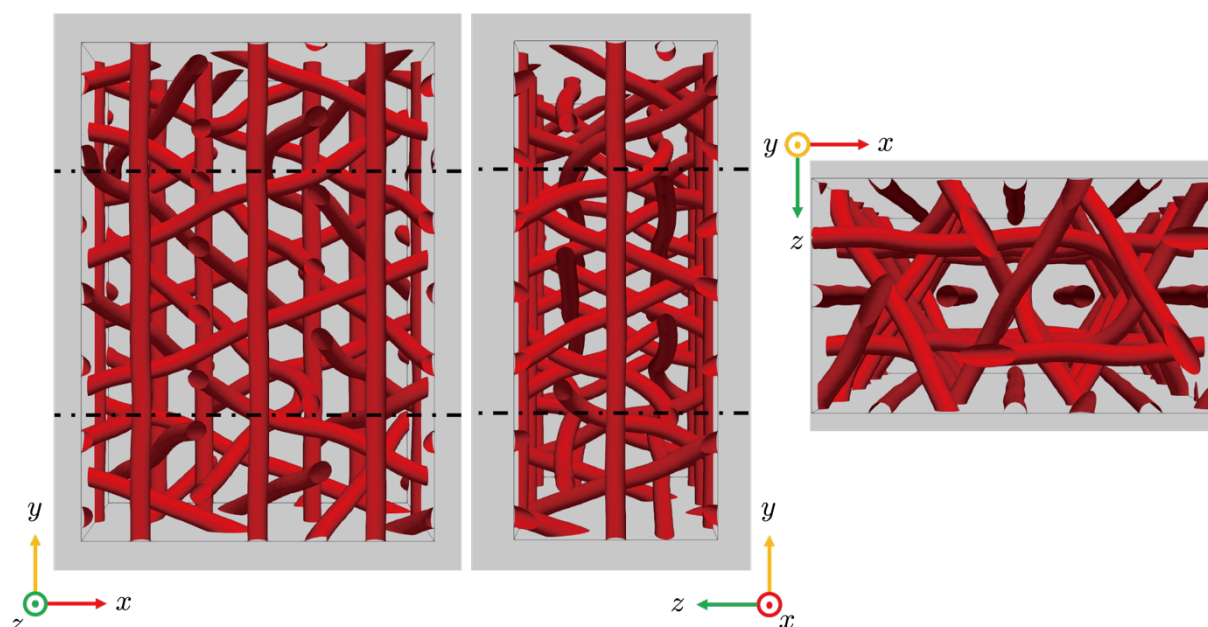
Figure 1: Structure of twin boundaries viewed from different directions. Depicted in red are disclination lines. Here the twin boundaries, highlighted by dot-dashed lines, are parallel to one of the {111} planes of the BP I lattices with different lattice orientations.

[1] H. M. Jin *et al.*, Sci. Adv. **6**, eaay5986 (2020).

Chiral topological states in flowing achiral nematics

S. Čopar [1], Ž. Kos [1,2], T. Emeršič [3,4,5] and U. Tkalec [3,4,6]

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[2] *Massachusetts Institute of Technology, Boston, Massachusetts, USA*
[3] *Jožef Stefan Institute, Ljubljana, Slovenia* [4] *Faculty of Medicine, University of Ljubljana, Ljubljana, Slovenia*
[5] *University of Chicago, Chicago, Illinois, USA*
[6] *University of Maribor, Ljubljana, Slovenia*

Nematic liquid crystals are known for supporting a variety of interesting topological structures in equilibrium – point defects, line defects, nonsingular solitons, periodic textures, and other related features of orientational order. These can be induced and controlled by external electric and optical fields, and most importantly, by confinement. However, subjecting the nematic to flow allows us to achieve additional structures that are not stable under understatic static equilibrium. Flow alignment under shear flow is a well known phenomenon of liquid crystals with appropriate viscosity parameters, and a nematic flow in a thin wide channel that enforces homeotropic alignment at the channel walls, exhibits a first order transition when flow rate is increased above a critical value. But before the flow-alignment transition, the nematic flow is unstable and undergoes a second order symmetry-breaking transition into a chiral state. This state is hard to achieve experimentally, as minor fluctuations in the velocity and orientational profile can trigger the flow-alignment transition, and was only recently first observed and described [1].

In this talk, I will demonstrate the experimental realization of the chiral-pretransitional state achieved by careful pressure control, and present the theoretical description and topological properties of this flow state.

[1] S. Čopar, Ž. Kos, T. Emeršič and U. Tkalec, *Microfluidic control over topological states in channel-confined nematic flows*, Nat. Commun. **11**, 977 (2020).

Optical solitons and chirality-enhanced nonlinear optical response in frustrated cholesterics

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[2] Department of Physics, University of Colorado, Boulder, Colorado.
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During the past 20 years, seminal works [1,2,3] by the groups of Prof. Assanto and Prof. Karpierz have established liquid crystals as an invaluable platform to study spatial optical solitons, which correspond to self-focused laser beams propagating without diffracting thanks to nonlinear optical effects. Indeed, liquid crystals are associated with a giant nonlocal response to external fields leading to the robust formation of accessible optical solitons called nematicons at beam powers of typically a few mW. Such optical solitons have mostly been studied in achiral nematic liquid crystals with a well-defined uniform far-field optical axis, in which the laser-induced perturbation of the molecular orientational field allows the compensation of diffractive effects. Although a few preliminary works [4,5] have shown the possibility of generating similar self-focused beams in chiral liquid crystals, the role of chirality in the nonlinear optical response of liquid crystals have not yet been fully elucidated.

In this contribution, I will present our recent contribution [6] to this topic: chirality can boost the non-linear optical response of frustrated cholesterics cells with homeotropic boundary conditions, thus leading to the formation of optical solitons at lower power than the nematicons of purely achiral samples. Such solitons are associated with an interesting bouncing pattern thanks to total internal reflections between the confining plates of the sample (see image below). I will explain the origin of this chirality-enhancement effect based on the formalism of Green functions, and if time allows I will also present additional applications of this novel physical effect.
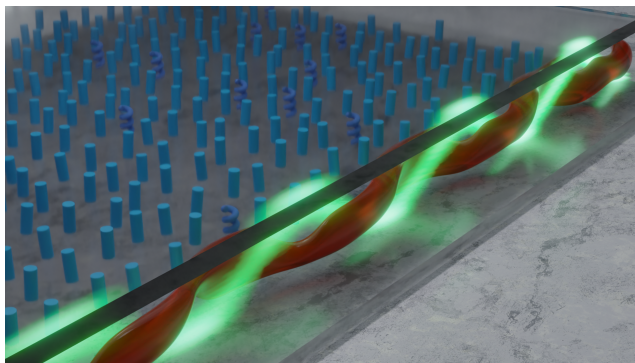

Figure: Simulated bouncing optical soliton (in green) in a frustrated cholesteric cell. The red domain corresponds to the part of the LC bulk with twist distortions of natural handedness.

[1] M. Peccianti, A. Dyadyusha, M. Kaczmarek, and G. Assanto, *Nat. Phys.* **2**, 737 (2006).
[2] *Nematicons: Spatial Optical Solitons in Nematic Liquid Crystals*, edited by G. Assanto, Wiley Series in Pure and Applied Optics (John Wiley & Sons, Hoboken, NJ, 2013).
[3] M. A. Karpierz, *Physical Review E* **66** (2002).
[4] F. A. Sala and M. A. Karpierz, *Opt. Express* **20**, 13923 (2012).
[5] A. Madani, J. Beeckman, and K. Neyts, *Opt. Commun.* **298-299**, 222 (2013).
[6] G. Poy, A. J. Hess, I. I. Smalyukh, and S. Žumer, *Phys. Rev. Lett.* **125**, 077801 (2020).

Pitch tuning induced by optical torque in heliconical cholesteric liquid crystals

G. Nava[2] ,F. Ciciulla[1],O. S. Iadlovska[3],O. D. Lavrentovich[3], F. Simoni1,
and L. Lucchetti[1]

[1] *Dipartimento SIMAU, Università Politecnica delle Marche, via Brecce Bianche, 60131 Ancona, Italy*
[2] *Dipartimento di Biotecnologie Mediche e Medicina Traslazionale, Università di Milano,Via Cervi 93 20090 Segrate (Mi),Italy*
[3] *Advanced Materials and Liquid Crystal Institute and Department of Physics, Kent State University, Kent, Ohio 44242, USA*

Heliconical cholesteric liquid crystals [1,2] are expected to be more sensitive to torque induced by light field with respect to conventional cholesterics, since their structure allows both bend and twist deformation. We report here a demonstration of tuning the helical pitch in heliconical cholesterics induced by an optical torque. According to our results, the helicoidal structure can be affected by an optical field orthogonal to the helix axis and the wavelength of the reflected light can be tuned from green to infrared by changing the power of the incident light. By varying the applied low-frequency electric field we demonstrate that tuning of the helical pitch is due to the additional optical torque acted on the molecular director by the light beam. Experimental observations are in agreement with expectations of the classical theory extended to include the effect of the optical field. A dual control of the helical pitch is achieved including both the low-frequency electric field applied along the helix axis and the optical field orthogonal to it [3].
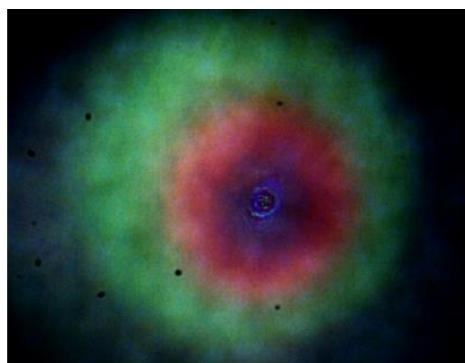
Figure 1: Sample appearance in reflection mode under the combined action of light and of a static electric field higher than the one required to totally unwind the helix.

Acknowledgements

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[2] J. Xiang, Y. Li, Q. Li, D. A. Paterson, J. M. D. Storey, C. T. Imrie, and O. D. Lavrentovich, Adv. Mater. 27, 3014 (2015).
[3] G. Nava, F. Ciciulla, O. S. Iadlovska, O. D. Lavrentovich, F. Simoni and L. Lucchetti, Phys. Rev. Res., 1, 033215 (2019).

Thursday, September 9

Chair	Matthias Lehmann
9:00	**PL4: Fumito Araoka** Mixtures of polar columnar liquid crystals – Does the domain size effect improve the switching speed?
9:40	**I8: Goran Ungar** Liquid crystal phase of counter-rotating staircases – A case of antiferrochirality
10:10	**O17: Xiangbing Zeng** Molecular origin of spontaneous macroscopic chirality in bicontinuous cubic and non-cubic phases
10:30	Poster pitches: P37-P39
10:40	Coffee break
Chair	Jan Lagerwall
11:10	**I9: Surajit Dhara** Smectic-like rheology and pseudolayer compression elastic constant of a twist-bend nematic liquid crystal
11:40	**O18: Maria Helena Godinho** Cellulose-based composites for colour-changing structural powders and inks
12:00	**O19: Per Rudquist** Confinement, twist elasticity and intrinsic chirality in micellar lyotropic nematic liquid crystals: A delicate balancing act
12:20	Poster pitches: P40-P45
12:40	Lunch
14:00	Online poster session (Gather.town)
15:30	Coffee break
Chair	Mojca Čepič
16:00	**I10: Alberta Ferrarini** Molecular features and polar nematic order
16:30	**O20: Davide Revignas** How shape polarity and concavity of mesogens affect Frank elastic constants
16:50	**O21: Jonathan Selinger** Director deformations, geometric frustration, and modulated phases in liquid crystals
17:10	**O22: Dina Jukić** Chiral polar bent-shape system: Why do gaps appear between certain relaxation modes?
19:30	Conference dinner

Mixtures of Polar Columnar Liquid Crystals
– Does the Domain Size Effect Improve the Switching Speed?

Fumito Araoka[1], Hiroya Nishikawa[1], Yuki Omata[1,2], and Daigo Miyajima[1]

[1] RIKEN Center for Emergent Matter Science, Wako, Japan
[2] Tokyo University of Science, Tokyo, Japan

In recent years, the study on polar dielectrics has received much attention due to their possibility for novel energy harvesting functions. In addition to the classical polar properties like ferroelectricity or piezoelectricity, new functional properties such as shift-current photovoltaic or flexo-photovoltaic effects [1] have been intensively investigated in various polar dielectric materials. Moreover, there have been emerging new polar dielectric systems, such as perovskites. Needless to say, polar liquid crystals are also attractive as a polar dielectric system for energy harvesting. For example, recently we have reported the shift-current photovoltaic effect in a sub-phthalocyanine-based polar columnar liquid crystal [2]. Although our material showed no polar switching property, its polarly aligned state served well for the shift-current photovoltaic effect. Thus, if the polar switching can be realized in addition to the shift-current photovoltaic property, it must be extremely fascinating and promising.

Up to now, we have synthesized couples of polar columnar liquid crystals based on our original molecular design with a phthalonitrile core assembled in the core-shell columnar architecture [3][4]. Some of them successfully exhibited the ferroelectric property, i.e. the remnant polarization and the polarization switching by field reversal. However, the common problem of these polar columnar liquid crystals is a trade-off between the switching speed and the spontaneous polarization - The spontaneous polarization can be stabilized through asymmetric molecular packing, but at the same time, the structural hinderance significantly increases the viscosity, resulting in the slow response with a switching time of typically more than 100 s. In this presentation, we will review some molecules with the same core design but with different ligands (Figure 1). Afterwards, the behaviours of the mixtures will be discussed. Interestingly, some of the mixtures showed significantly improved switching speeds compared to only the component materials. By polarization microscopy, X-ray diffractometry and differential scanning calorimetry, it looks to be likely attributed to the domain size effect induced through the nanoscopic phase segregation. In fact, the similar effect is known in inorganic ferroelectrics - the smaller the ferroelectric domains, the faster the responses. Thus, it is considered that the similar strategy may be also applicable to improve the switching in the polar liquid crystal systems.
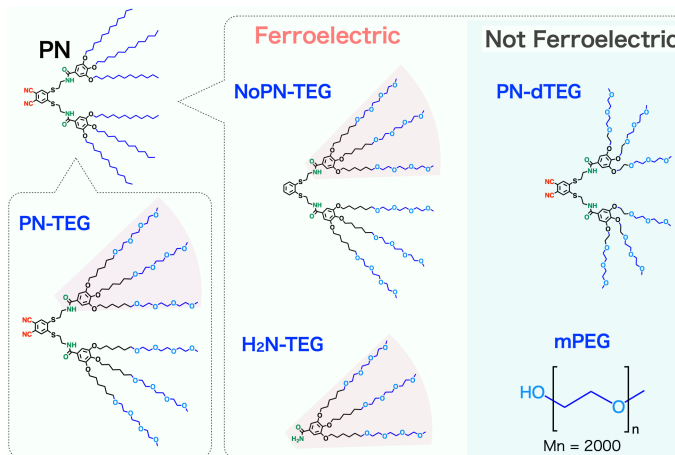

Figure 1: Our molecular design for the polar columnar liquid crystals

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[2] Cheng Zhang, Kyohei Nakano, Masao Nakamura, Fumito Araoka, Keisuke Tajima, and Daigo Miyajima, J. Am. Chem. Soc. **142**, 3326 (2020).
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[4] Fumito Araoka, Morio Isoda, Daigo Miyajima, Inseon Seo, Masahito Oh-e, Takuzo Aida, and Hideo Takezoe, Adv. Electron. Mater. **3**, 1600503 (2017).

Liquid crystal phase of counter-rotating staircases – A case of antiferrochirality

Ya-xin Li[1,2], Yi-nan Xue[1], <u>Goran Ungar</u>[1,2], Rui-bin Zhang[2], Xiang-bing Zeng[2], Hong-fei Gao[3], Xiao-hong Cheng[3], Feng Liu[1], Kutlwano Gabana[2] and Gillian A. Gehring[2]

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2 University of Sheffield, Sheffield, UK
3 Key Laboratory of Medicinal Chemistry from Natural Resources, Kunming, P. R. China

Helical structures continue to inspire, and there is considerable temptation to attribute helicity to columnar LCs. While short isohelical sequences are undoubtedly present, and longer ones in chiral or chiral-doped compounds, the order is only short-range, equivalent to a paramagnet without or with field, respectively. However, here we report a confirmed example of a true LC phase, not a soft crystal, of achiral compounds consisting of columns, each being a long-range homochiral helix [1]. Long-range periodicity and isochirality are maintained by intercolumnar interaction. This orthorhombic LC, spacegroup *Fddd*, is discovered in compounds with either bent or straight rod-like pi-conjugated cores (see Fig. 1), and is subsequently found in other systems, including polymers. There are 4 right and 4 left-handed ribbons or star-profiled columns per unit cell. The structure is equivalent to an antiferromagnet with twist replacing spins. A theory based on interacting quadrupoles confirms this structure as energetically favoured over alternatives. Although, due to cancellation, the current *Fddd* phase has no overall chirality, the findings open a new approach to homochirality in achiral compounds.
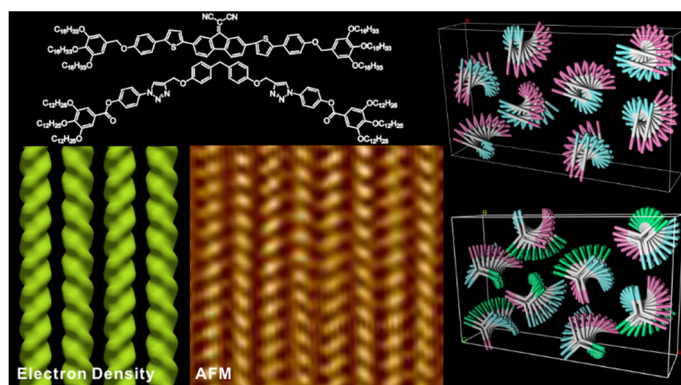

Figure 1: Top left: Some of the compounds displaying the *Fddd* phase. Bottom left: Electron density map (green) and AFM phase contrast image of the (110) plane, showing alternating left- and right-twisted columns. Right: schematic of packing of straight-core (top) and bent-core molecules (bottom) [1].

[1] Y. X. Li et al. *Nat. Chem.; In Review* http://dx.doi.org/10.21203/rs.3.rs-256979/v1

Molecular Origin of Spontaneous Macroscopic Chirality in Bicontinuous Cubic and Non-cubic Phases

Huanjun Lu,[1,2] Yaxin Li,[1] Xiangbing Zeng,[1] Goran Ungar,[1,3] Christian Dressel[4] and Carsten Tschierske[4]

[1] Department of Materials Science and Engineering, University of Sheffield, UK.
[2] College of Chemistry, Chemical Engineering and Materials Science, Soochow University, China.
[3] State Key Laboratory for Mechanical Behaviour of Materials, Shanxi International Research Center for Soft Materials, Xi'an Jiaotong University, Xi'an, China.
[4] Institute of Chemistry, Martin-Luther-University Halle-Wittenberg, Halle, Germany.

The discovery of spontaneous formation of chirality at macroscopic scale in bicontinuous cubic [1] and isotropic [2] phases of achiral polycatenar compounds has challenged many of our previous perceptions about the structures of such phases. Upon careful examination of a series of bicontinuous phases formed by polycatenar compounds (chiral or achiral, cubic [3] or non-cubic [4]), by a combination of diffraction, microscopy and spectroscopy methods, a universal mechanism through which achiral polycatenar compounds are able to produce such macroscopic chirality has been revealed. This mechanism includes at the molecular level the formation of local chiral column-like segments with a slow twist in molecular direction along them. The propagation of homochirality throughout the network occurs through twist-sense synchronization at network junctions, as well as through inter-network interactions.
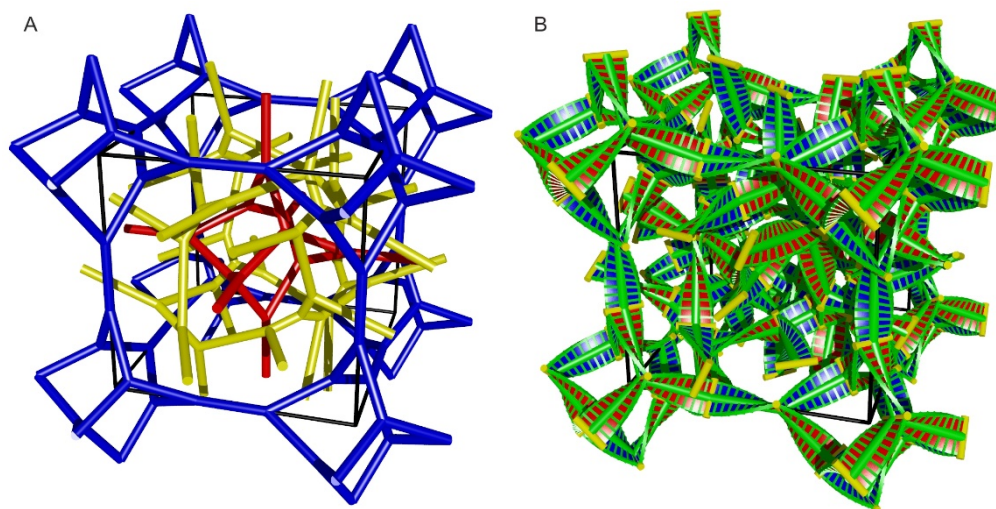

Figure 1. A new model of the triple network chiral bicontinuous cubic phase. A. The three interpenetrating networks, coloured red, yellow and blue respectively. B. The corresponding ribbon model showing twisting of molecular direction in all three networks.[3]

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Smectic-like rheology and pseudolayer compression elastic constant of a twist-bend nematic liquid crystal

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In twist-bend nematic (N_{TB}) liquid crystals (LCs), the director (mean molecular orientation) exhibits heliconical structure with nanoscale periodicity. On the mesoscopic scale, N_{TB} resembles layered systems (like smectics) without a true mass density wave, where the helical pitch is equivalent to a "pseudolayer." We study rheological properties of a N_{TB} phase and compare the results with those of a usual smectic-*A* phase. Analysing the shear response and adapting a simplified physical model for the rheology of defect-mediated lamellar systems, we measure the pseudolayer compression elastic constant B_{eff} of the N_{TB} phase from the measurements of the dynamic modulus $G^*(\omega)$. It is found that B_{eff} of the N_{TB} phase is in the range of 10^3–10^6 Pa and it follows a temperature dependence, $B_{eff} \sim (T_{TB} - T)^2$, as predicted by the recent coarse-grained elastic theory. Our results show that the structural rheology of N_{TB} LCs is strikingly similar to that of the usual smectic LCs, although the temperature dependence of B_{eff} is much faster than that of smectic LCs as predicted by the coarse-grained models.
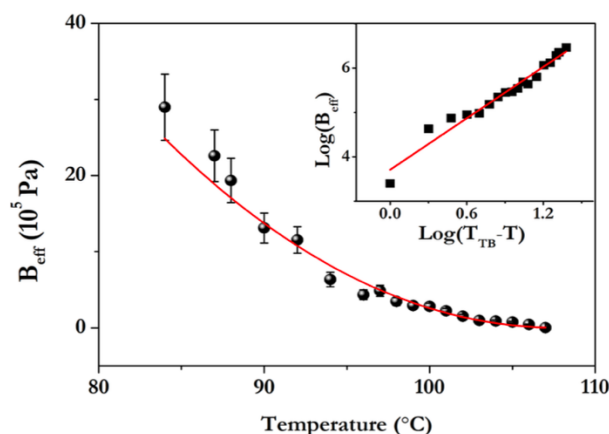
Figure 1: Temperature dependence of effective elastic compressional modulus B_{eff}. The solid line is a theoretical fit to the equation $B_{eff} \sim (T_{TB} - T)^\alpha$, where $\alpha = 2.0 \pm 0.1$. Inset: Log-log scale.

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Cellulose-based composites for colour-changing structural powders and inks

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Thermotropic and thermochromic cellulose-based systems are well known and very much reported in literature [1, 2]. Less studied are cellulose-based dispersed liquid crystals [3]. In this work we present the study of inks made from a cellulose-based thermochromic composite material. The composite is formed by a matrix of a left-handed n-butyric acid ester of hydroxypropylcellulose (BPC) with cholesteric liquid crystals of small left and right-handed molecules (Ch). The cellulose derivative and the Ch compounds show reflection bands in the visible region, at room temperature. We show that the reflection wavelengths vary with temperature and the amount of the Ch in the composite. For certain Ch+BPC concentrations cholesteric micro and submicron droplets develop with colour-changing caps different from de bulk (Figure 1). The system was investigated with a polarised optical microscope (POM), working in transmission and reflection modes, scanning electron microscopy (SEM) and atomic force microscopy (AFM) The reflection spectra was acquired as a function of temperature and cellulose derivative concentration. The results obtained indicate that cellulose-based coloured composites are good candidates for the production of structural multi-coloured powders and inks.
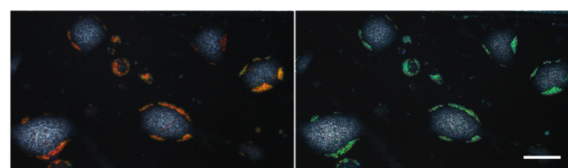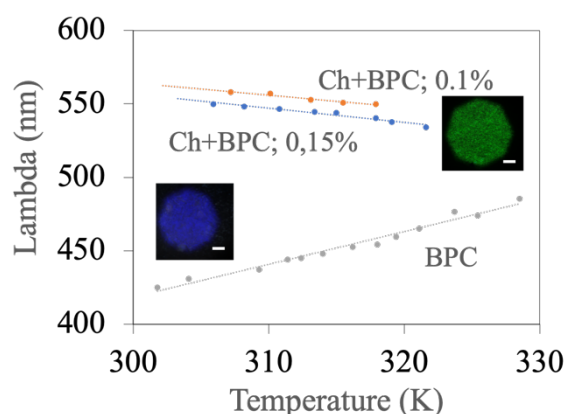

Figure 1. Wavelength of maximum selective reflection as a function of temperature for mixtures of Ch and BPC. Photos correspond to POM reflection and transmission images for different concentrations of the cholesteric components. Scale bars represent 100 µm.

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Confinement, twist elasticity and intrinsic chirality in micellar lyotropic nematic liquid crystals: A delicate balancing act

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Lyotropic nematic liquid crystals (LLCs) are exceptional in their viscoelastic behavior, for example, displaying an extreme softness to twist deformation [1]. This often leads to chiral director configurations under achiral confinement despite the lack of intrinsic chirality of the LLC. In the case of cylindrical confinement with homeotropic anchoring, the twisted escaped radial (TER) and the twisted polar (TP) configurations are the two reflection-symmetry breaking director configurations typically observed [2].

Introducing intrinsic chirality by the addition of a chiral dopant, various new structures and phenomena are observed enabling a comprehensive study of the delicate interplay between confinement, twist elasticity and intrinsic chirality in a micellar LLC [3]. Comparison of the effects of intrinsic chirality on the defect-free TER configuration, and on the TP configuration incorporating two half-unit twist disclination lines, is examined. In case of the TER configuration, a doubly twisted escaped radial (DTER) configuration is found in which the escape direction spirals along the capillary diameter. For the TP configuration, topological constraints promote stable heterochiral systems even in the presence of a small amount of chiral dopant, with unusual regions containing multiple reversals of handedness between homochiral domains. At moderate dopant concentrations the TP structure becomes homochiral. At high dopant concentrations, the induced cholesteric pitch is much smaller than the diameter of the capillary and the cholesteric fingerprint structure develops.
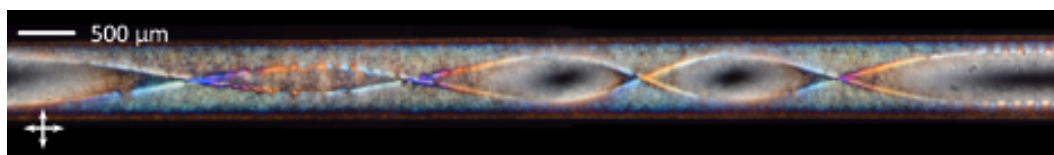
Figure 1: Twisted polar (TP) structure of a lyotropic nematic under cylindrical confinement with a double helix of two twist disclination lines. The figure shows smooth double helix domains and regions with closely spaced kinks in the two disclination lines.

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Molecular features and polar nematic order

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Among the recent discoveries of novel nematic phases, the most exciting is probably that of polar order, which was found in low molar mass mesogenic systems upon cooling from the conventional nematic [1-3]. This discovery raised several questions, concerning the nature of the phase transition and the structure of the polar phase, as well as the molecular factors that promote its formation. The latter point is crucial for the development of new materials exhibiting polar order at temperatures suitable for applications. So far, polar nematic order was observed at high temperature in a very limited range of compounds, with the common feature of a high electric dipole moment. However, a strong dipole is also present in the molecules of most conventional nematics; so, although probably necessary, this is not sufficient to stabilize polar order. It was proposed that a wedge shape could be a distinctive molecular feature; however, in this regard it is not easy to detect a clear difference between structurally related compounds that exhibit or do not exhibit the polar nematic organization. Indeed, systematic synthetic investigation has shown that this change in behaviour can be determined by tiny changes in the molecular structure [4,5].

Along the years, the existence of a polar nematic phase was addressed by microscopic theories and computer simulations, with somewhat controversial results. No evidence of this phase was found for elongated particles [6,7], but a stable ferroelectric phase was observed for tapered shapes [8]. Polar nematic order was found also by a lattice model including polar interactions between neighboring sites and polar order-local splay coupling, and it was associated with the emergence of spontaneous splay [9]. Thus, a relationship with softening of the splay elastic constant was proposed [10,11]. Here, the role of molecular features and the mechanism behind the onset of nematic ordering will be discussed using models developed in our group [12,13].

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How shape polarity and concavity of mesogens affect Frank elastic constants

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Classical microscopic theories [1–4] of nemato-elasticity, typically based on the assumptions of rod-like mesogens and unperturbed orientational distribution function, successfully reproduce the textbook experimental trend of Frank elastic constants [5] (monotonic increase with increasing order, $K_{33} > K_{11} > K_{22}$). However, recent interest in the continuously expanding variety of nematic systems [6–9] has brought to light several examples of unconventional elasticity. Among these we can list bent molecules [10, 11], supramolecular polymers [12, 13] and actin-based filaments [14, 15]. All these elastic anomalies pose a serious challenge to the traditional theoretical approach to nemato-elasticity [12, 13, 16]. Previous attempts to tackle such challenge include a few studies dealing with the specific case of particles of polar symmetry [17–20] and some efforts to take into account the flexibility of polymeric chains [21]. Although for specific cases these attempts do overcome the limitations of classical theories, a general theoretical framework is still missing.

We recently proposed [22] a model applicable to arbitrarily shaped objects and to arbitrarily deformed nematics. The main novelty is the use of a non-local orientational distribution function which accounts for the coupling of mesogen morphology and director distortions. The predicted elastic constants are strongly sensitive to particle morphologies and, for non-convex ones, exhibit unconventional features.

Here we will present the results for model particles for which we can tune some morphological parameters such as the shape polarity and chirality. We will show how different molecular features have different effects on the macroscopic elastic properties and we will evidence the role of concavity on the deviation from the classical rod-like behavior.

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Director Deformations, Geometric Frustration, and Modulated Phases in Liquid Crystals

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We analyze modulated phases in liquid crystals, using the concept of four fundamental modes of director deformation: twist, bend, splay, and a fourth mode related to saddle-splay [1,2]. Each mode is coupled to a specific type of molecular order: chirality, polarization perpendicular and parallel to the director, and octupolar order. When the liquid crystal develops one type of spontaneous order, the ideal local structure becomes nonuniform, with the corresponding director deformation. In general, the ideal local structure is frustrated; it cannot fill space. As a result, the liquid crystal must form a complex global phase, which may have a combination of deformation modes, and may have a periodic array of defects. Thus, the concept of an ideal local structure under geometric frustration provides a unified framework to understand the wide variety of modulated phases [3].

Deformation	Deformation considering $\hat{n} \leftrightarrow -\hat{n}$	Mathematical object	Corresponding molecular order	Achievable global phases (nematic)	Achievable global phases (smectic-A)
Twist $T = \hat{n} \cdot \nabla \times \hat{n}$	Twist $T = \hat{n} \cdot \nabla \times \hat{n}$	Pseudoscalar	Chiral order parameter	Cholesteric Blue phases	Twist grain boundary Helical nanofilaments
Bend $\boldsymbol{B} = \hat{n} \times \nabla \times \hat{n}$	Bend $\boldsymbol{B} = \hat{n} \times \nabla \times \hat{n}$	Vector $\perp$ to $\hat{n}$	Polarization $\boldsymbol{P}_\perp$	Twist-bend N_{TB} Splay-bend N_{SB}	Possible lattice of edge dislocations
Splay scalar $S = \nabla \cdot \hat{n}$	Splay vector $\boldsymbol{S} = \hat{n}(\nabla \cdot \hat{n})$	Vector $\parallel$ to $\hat{n}$	Polarization $\boldsymbol{P}_\parallel$	Splay nematic N_S	Spherical shells
Δ_{ij}	$\Delta_{ij} n_k$	Tensor of rank 3	Octupolar order parameter	Not yet studied	Helical nanofilaments

Table 1: Director deformations, corresponding molecular order, and achievable phases

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Chiral polar bent-shape system: Why do gaps appear between certain relaxation modes?

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In the chirally doped antiferroelectric system made of bent-shaped compounds, two phases with the same symmetry exist: the $\mathrm{SmAP_A^*}$ phase, where the dopant induces a small anticlinic tilt, and the $\mathrm{SmC_AP_A^*}$ phase, which is genuinely anticlinicaly tilted, even without the presence of the chiral field [1]. In addition, the two phases continuously develop one to another. To determine the temperature ranges of the $\mathrm{SmAP_A^*}$ and the $\mathrm{SmC_AP_A^*}$ phase, relaxation modes of the system were analysed [2]. The temperature ranges were deduced from the temperature dependence of the Soft mode, which has a minimum that indicates the softening of the chiraly doped sample, although the mode does not behave critically as it would in a system without the dopant. Further analysis of the relaxation modes revealed that the modes are either related to the changes of amplitude or to the changes of phase of the stable tilts and polarizations. This is referred to as character of the mode and is illustrated in Fig. (a), where amplitude modes are color-coded red and phase modes are color-coded blue. Additionally, relaxation modes occur in pairs of opposite chiralities, shown in Fig. (b), which is indicated by the appearance of gaps between amplitude modes in the temperature range of the $\mathrm{SmAP_A^*}$ phase.

To compare the predicted behaviour with potential experimental measurements, the effects of fluctuations related to different relaxation modes on the birefringence of the sample is presented.
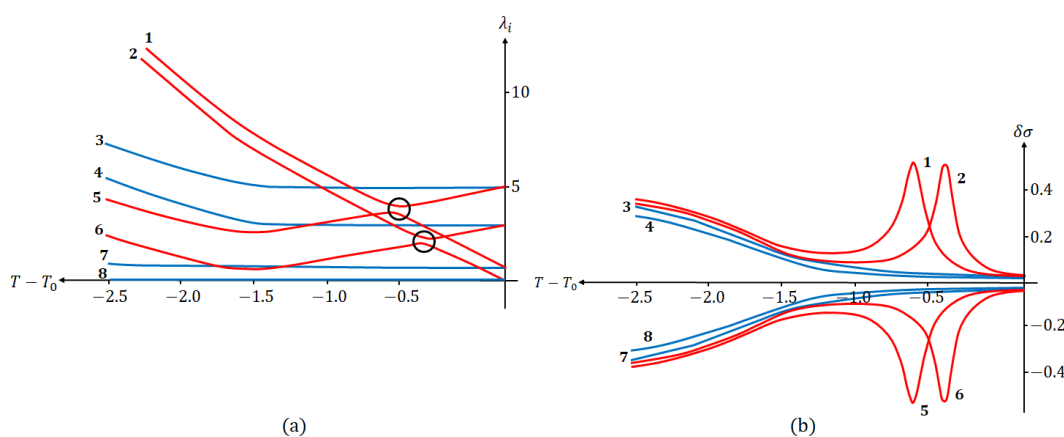

Figure 1: (a) Amplitude(red) and phase(blue) relaxation modes in the vicinity of $\mathrm{SmAP_A^*} \leftrightarrow \mathrm{SmC_AP_A^*}$ phase transitions. Circles indicate the gaps which appear between the amplitude modes of opposite chiralities. (b) Chiral properties of the relaxation modes.

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Friday, September 10

Chair	Oleg Lavrentovich
9:00	**PL5: Sofia Kantorovich** The effects of particle shape on the self-assembly
9:40	**I11: Alexey Eremin** Magnetic tilting in nematic liquid crystals driven by self-assembly
10:10	**O23: Melvin Küster** Ferromagnetic nematics in rotating and oscillating magnetic fields
10:30	Coffee break
Chair	Simon Čopar
11:00	**I12: Vladimir Chigrinov** Photoaligned ferroelectric liquid crystals: new electrooptical modes
11:30	**O24: Mikhail Osipov** Competition between ferroelectric ordering and elastic instability in polar nematic LCs. Why the ferromagnetic state may be stable while the ferroelectric one is not.
11:50	**O25: Oxana Prishchepa** Periodic structures of linear defects in cholesteric layer with conical-planar anchoring under electric field
12:10	Closing Ceremony
12:30	Lunch
14:00	End of the conference

The effects of particle shape on the self-assembly

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Stable dispersions of magnetic colloidal particles with sizes ranging from nanometers to couple of microns have been actively studied for several decades and the interest to them seems to keep growing. Such an attention to these systems is paid because of several reasons: they are biocompatible, can be remotely controlled by external magnetic fields and new synthesis techniques enable a rich variety of particle morphologies.

In classical magnetic fluids with spherical polydisperse nanoparticles, dominating dipolar interactions typically limit the structural complexity of their aggregates to linear arrangements, namely chains, rings and branched structures.

In this contribution I will show, how to either alter the shape of magnetic particles or their internal structure in order to extend dramatically the topology and properties of their suspensions. In particular I will focus on magnetic cubes, magnetic Janus particles, soft magnetic colloids and magnetically anisotropic nanoparticles. I will show how lattices, branched clusters of staggered chains, compact clusters, linear chains, and non aggregated configurations can be formed and interconverted reversibly in a controlled way. I will also discuss how adding an active component to magnetically anisotropic particles leads to unique properties. The results gathered in this presentation demonstrate that fundamentally new possibilities for responsive magnetic materials can arise when we step away from conventional dipolar hard spheres.

Magnetic Tilting in Nematic Liquid Crystals driven by Self-Assembly

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Self-assembly is one of the crucial mechanisms allowing to design multifunctional materials. Soft hybrid materials contain components of different nature and exhibit competitive interactions which drive self-organisation into structures of a particular function. Here we demonstrate the manipulation of the optical properties of a soft colloidal LC-hybrid material using a delicate balance between the topologically-assisted colloidal self-assembly of magnetic nanoparticles (MNPs) and the anisotropic molecular interactions. The hybrid material is based on the 5CB nematic liquid crystal with dispersed dendronised cobalt ferrite MNPs with a core size of 4.6 nm [1]. The key feature in the design of these materials is the functionalization of the MNPs, allowing an effective coupling between the magnetic particles and the LC matrix. Using magneto-, electrooptical and X-ray studies, we demonstrate that the ferronematic hybrid materials with dendron-functionalized MNPs show a magnetically-induced tilt of the nematic director. We explain this tilt by the formation of mesoscopic, topologically-driven self-assembled chain-like structures of MNPs stabilized through the long-range, director-mediated interactions [2]. The magnetic alignment of these structures is responsible for the reorientation of the liquid crystal director.

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Ferromagnetic nematics in rotating and oscillating magnetic fields

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Soft magnetic materials, such as magnetic fluids, gels and elastomers, have recently come into focus of intensive research. The ability to easily manipulate optical and mechanical properties makes them essential components for designing intelligent materials. Recently, Mertelj et al. demonstrated that dispersions of magnetic nano-platelets in liquid crystals could exhibit ferromagnetic order [1,2]. Liquid crystalline order is expected to profoundly affect the dynamics of the magnetic particles, which is still not fully understood. Here, we report the study of magnetization dynamics and the magnetomechanical effect of a colloidal dispersion of barium hexaferrite nano-platelets in rotating and oscillating magnetic fields. Magnetic relaxation was studied using AC susceptometry and magnetization measurements in a rotating magnetic field in a frequency range from 0.1 Hz - 9 kHz and for field amplitudes up to 5 mT. The magnetomechanical effect is studied in a spherical cavity suspended on a torsional pendulum. We performed the studies in a wide range of concentration, from the diluted isotropic suspension to the nematic state. In those suspensions, we observe a high-frequency magnetic relaxation mode related to the diffusion of the single particles and a low-frequency mode, which can be attributed to the cooperative motion of the magnetic nanoparticles (MNPs). The wide size distribution of the particles results in a polydisperse Debye behaviour.

Our studies show that the magnetomechanical torque follows the same frequency behaviour as the loss part of the AC susceptibility χ''. Moreover, the conversion efficiency of the magnetic torque into the mechanical is particularly strongly pronounced in our system since the Néel relaxation mechanism is suppressed. The origin of the magnetomechanical torque is the vortex flow sustained by rotating MNPs. We characterise this flow using a particle tracking technique.

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Photoaligned ferroelectric liquid crystals: new electrooptical modes

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Photoalignment and photopatterning has been proposed and studied for a long time [1]. Light is responsible for the delivery of energy as well as phase and polarization information to materials systems. It was shown that photoalignment azodye materials could provide high quality alignment of molecules in a liquid crystal (LC) cell. Over the past years, a lot of improvements and variations of the photoalignment and photopatterning technology has been made for display and photonics applications. In particular, the application of this technology to active optical elements in optical signal processing and communications is currently a hot topic in photonics research [2].

We will demonstrate new electrooptical modes in photoaligned FLC: (i) Electrically Suppressed Helix (ESH) mode; (ii) Deformed Helix Ferroelectric (DHF) mode; (iii) bi and multistable FLC modes; (iv) Switchable Diffraction Grating (SDG) mode; (v) Kerr effect mode. Possible applications in microdisplays, shutters, lenses, light attenuators etc will be also considred [2]

Acknowledgements

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Competition between ferroelectric ordering and elastic instability in polar nematic LCs. Why the ferromagnetic state may be stable while the ferroelectric one is not.

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It has been known for a long time that a mean-field molecular theory can easily predict a proper ferroelectric ordering in the nematic phase composed of strongly polar molecules although this has never been observed experimentally. A possible explanation is that strongly polar particles have a tendency to form chains rather than to establish a ferroelectric order [1]. On the other hand chain formation has also not been observed experimentally even in strongly polar nematics. Thus it remains unclear why the ferroelectric state is not observed in nematics.

A molecular field theory has been used to calculate the polar order parameter and the splay elastic constant in the nematic phase composed of polar uniaxial molecules. It has been shown that polar intermolecular interactions result in a polar correction to the splay elastic constant which is increasing in the pretransition region when the temperature approaches the point of virtual transition into the ferroelectric nematic phase. Moreover, the correction formally diverges at the virtual phase transition temperature and thus the splay constant vanishes at some point above the transition into the ferroelectric state. As a result the homogeneous nematic phase looses its stability with respect to an inhomogeneous distribution of the director and the polar order parameter and the system undergoes a transition into the splay-bend phase or some other modulated locally polar phase.

This behaviour is rather universal and is related to the flexoelectric effect. Thus the homogeneous ferroelectric nematic phase can never be stable because it is always pre-empted by the elastic instability leading to the formation of the modulated phase regardless of the particular molecular structure. A similar instability occurs also in bent-core nematics [2,3] but the present theory is restricted to the case of uniaxial molecules.

Recently a homogeneous ferromagnetic state has been observed experimentally in nematics composed of disc-like molecules [4]. One notes that this is not in contradiction with the above mentioned results as the magnetization has a different symmetry compared with the polarization. Polarization is a polar vector while magnetization is an axial vector which is not linearly coupled with spay and bend polar vectors in a nonchiral sytems. We explain in detail why the polar correction to the splay constant is relatively small and does not grow upon approaching the transition into the ferromagnetic nematic phase which in principle does not violate the stability of the ferromagnetic state.

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[2]. Shamid SM, Dhakal S, Selinger JV. Phys Rev E.87, 052503 (2013).
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[4]. A. Mertelj and D,Lisjak, Liquid Crystal Reviews, 5, 1, (2017).

Periodic structures of linear defects in cholesteric layer with conical-planar anchoring under electric field

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Cholesteric liquid crystals (CLCs) having a helicoid structure with a period p attract attention due to their ability to form the various textures in electric field. The cholesteric structure depends mainly on the anchoring conditions at the interface. Now, CLC structures with homeotropic, planar or hybrid homeo-planar boundary conditions have been studied in detail [1,2]. Recently, new director configurations in cholesteric layers with conical-planar anchoring have been investigated for different ratios of the layer thickness d to the helix pitch p_0 [3]. In present paper we consider the periodic structures in cholesteric layer with conical-planar anchoring and their transformation under applied electric field. The experimental findings are supported by the calculation data. The given structures are the set of alternating over- and under-twisted defect lines whose azimuthal director angles differ by 180°. The U^+- and U^--defects of periodicity, which are the smooth transition between the defect lines, are observed at the edge of electrode area. The growth direction of defect lines forming a diffraction grating can be controlled by applying a voltage in the range of $0 \leq V \leq 1.3$ V during the process (Fig.1) [4]. Resulting orientation and distance between the lines don't change under voltage. However, at $V>1.3$ V U-defects move along the defect lines away from the electrode edges, and finally, the grating lines collapse at the cell's centre. These results open a way for the use of such cholesteric material in applications with periodic defect structures where a periodicity, orientation, and configuration of defects should be adjusted.
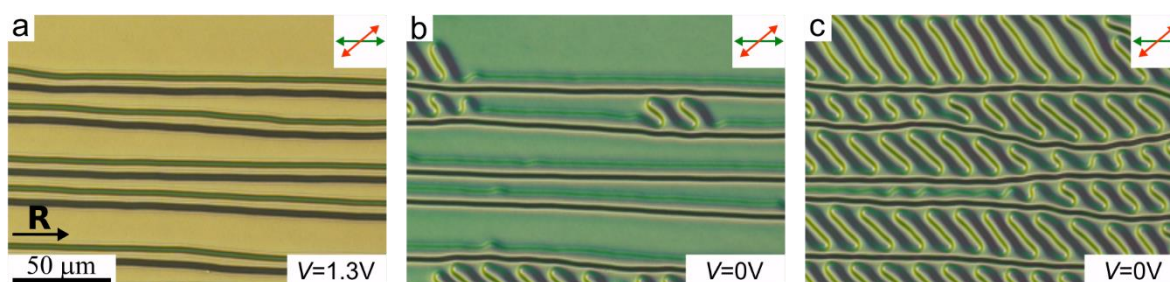

Figure 1: POM photos of CLC layer with the defect lines formed nearly parallel to the rubbing direction **R** under V = 1.3 V (a) and in 9.2 sec (b), 46.8 sec (c) after switching off the field. The analyzer is oriented to the polarizer at 40° angle [4]

[1] P. Oswald, & P. Pieranski, Nematic and cholesteric LC: concepts and physical properties illustrated by experiments, (Taylor & Francis, Boca Raton, 2005), pp. 618.
[2] J. Baudry, et al. Liq. Cryst., **21**, 893 (1996).
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[4] O. Prishchepa, et al., Scientific Reports, (2021) doi:10.1038/s41598-021-87854-z.

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Emergence of flexoelectric polarization in liquid-crystalline elastomers cross-linked under asymmetric deformation.

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Emergence of flexoelectric polarization in liquid crystalline elastomers composed of cholesterol-derived mesogens prepared in cross-linking under asymmetric deformation, such as horseshoe-like deformation and uniaxial deformation with slay distortion were investigated. X-ray diffractometry revealed that the orientational order partially remained about $S = 0.15 \sim 0.2$ even in the temperature region of the isotropic phase designated tentatively as the pseudo-isotropic phase, and also that bend and/or splay distortion occurred along the depth direction in the elastomers. The emergence of polarization was confirmed above the SmA* to pseudo-isotropic phase transition temperature whereas no polarization appeared in the SmA* phase. The electric charge due to the polarization increased with increasing temperature in the pseudo-isotropic phase and attained at 1500 pC, though almost no charge appeared in the SmA* phase. We tentatively conclude that macroscopic polarization due to the flexoelectric effect emerged and fixed in the elastomers within cross-linked bend and/or splay distortion in the horseshoe-like deformed elastomers.

[1] K. Hiraoka et al., Liquid Crystals **47**, 1535-1545 (2020).

New example of a ferroelectric nematic phase material

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The recent discovery of the ferroelectric nematic phase (N_F) opens completely new perspectives in the science and technology of nematic liquid crystals (NLCs). The long-range directional correlation of strong molecular dipoles in the N_F phase gives rise to its high spontaneous electric polarization, the magnitude of which is in the order of several 10^{-6} C cm^{-2} and the direction of which is highly responsive to the action of external electric fields [1]. So far, this new N_F phase was reported for three liquid-crystalline materials, in two of them [2, 3] the N_F phase directly follows a conventional nematic phase (N) at lower temperatures and a third material with a direct isotropic – N_F transition [4].

We now report another example of a ferroelectric NLC where the N and N_F phases are separated by an intermediate nematic phase, N_x. The molecular structure (Fig. 1a) includes several fluorinated building blocks, an oxane ring and a terminal cyano group, all of which contribute to the strong molecular dipole moment of about 12 D along the long molecular axis. The monotropic N_F phase is confirmed by its high dielectric permittivity (Fig. 1b) and by the presence of ferroelectric domains with opposite twist sense and polar electro-optic response (Fig. 1c). We present a thorough characterization of this fascinating new material including polarization measurements as well as X-ray and electro-optic studies.
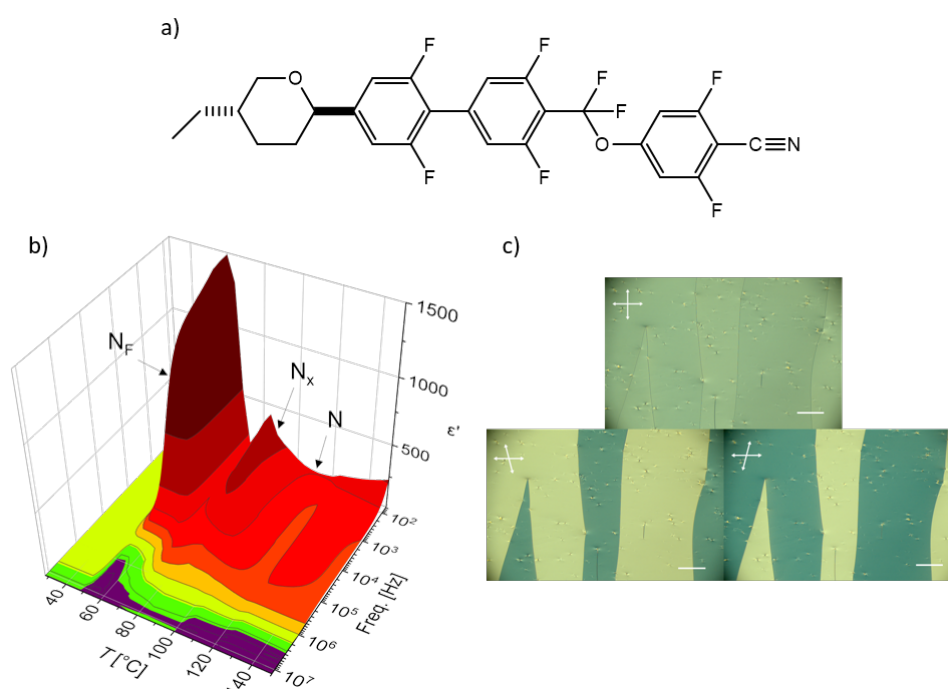

Figure 1: Selected features of the new N_F material: (a) molecular structure, (b) dielectric relaxation spectrum, and (c) domains of opposite twist sense (scale bars: 200 µm).

[1] X. Chen, E. Korblova, D. Dong *et al.*, Proc. National Acad. Sci. **117**, 14021 (2020).
[2] N. Sebastián, L. Cmok, R. J. Mandle *et al.*, Phys. Rev. Lett. **124**, 037801 (2020).
[3] H. Nishikawa, K. Shiroshita, H. Higuchi *et al.*, Adv. Mater. **29**, 1702354 (2017).
[4] A. Manabe, M. Bremer, and M. Kraska, Liq. Cryst., *in press* (2021).

Surface alignment of ferroelectric nematic liquid crystals

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[2] *Dipartimento SIMAU, Università Politecnica delle Marche, via Brecce Bianche, 60131 Ancona, Italy.*
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The success of nematic liquid crystals in displays and optical applications is due to the combination of their optical uniaxiality, fluidity, elasticity, responsiveness to electric fields and controllable coupling of the molecular orientation at the interface with solid surfaces. The discovery of a polar nematic phase [1-5] opens new possibilities for liquid crystal-based applications, but also requires a new study of how this phase couples with surfaces. Here we explore the surface alignment of the ferroelectric nematic phase by testing different rubbed and unrubbed substrates (Figure 1) that differ in coupling strength and anchoring orientation and find a variety of behaviors - in terms of nematic orientation, topological defects and electric field response - that are specific of the ferroelectric nematic phase and can be understood as a consequence of the polar symmetry breaking. In particular, we show that by using rubbed polymer surfaces it is easy to produce cells with a planar polar preferential alignment and that cell electrostatics has a remarkable effect on the overall homogeneity of the ferroelectric ordering.
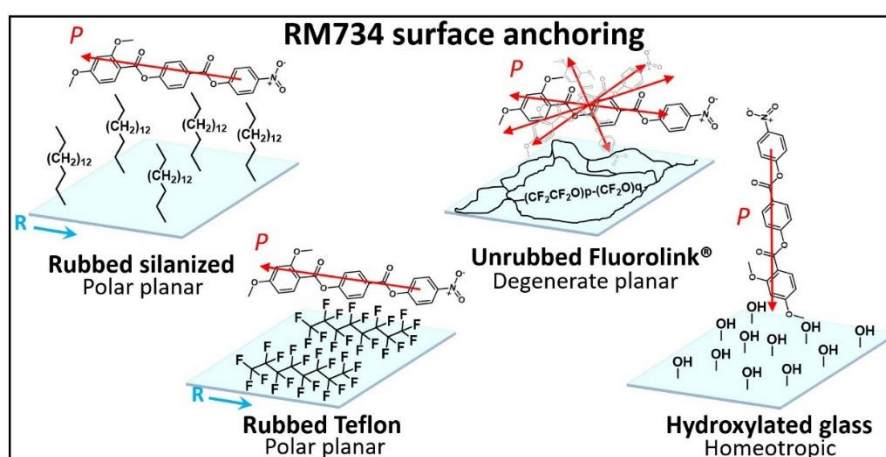

Figure 1: Summary of the different surfaces studied in the present work

[1] R. J. Mandle, S. J. Cowling, and J. W. Goodby, Phys. Chem. Chem. Phys. **19**, 11429-11435 (2017).
[2] A. Mertelj, L. Cmok, N. Sebastian, R. J. Mandle, R. R. Parker, A. C. Whitwood, J. W. Goodby, M. Copic, Phys. Rev. X **8**, 041025 (2018)
[3] H. Nishikawa, K. Shiroshita, H. Higuchi, Y. Okumura, Y. Haseba, S. Yamamoto, K. Sago, H. Kikuchi, Adv. Mater. **29**, 1702354 (2017).
[4] N. Sebastian, L. Cmok, R. J. Mandle, M. Rosario de la Fuente, I. Drevenšek Olenik, M. Čopič, A. Mertelj, Phys. Rev. Lett **124**, 037801 (2020).
[5] X. Chen, E. Korblova, D. Dong, X. Wei, R. Shao, L. Radzihovsky, M. Glaser, J. Maclennan, D. Bedrov, D. Walba, N.A. Clark, Proc. Natl. Acad. Sci. U.S.A. **117**, 14021-14031, (2020)

Electrowetting phenomena in a polar nematic liquid crystal

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The recent discovery of polar nematic materials [1,2] revealed that highly fluidic materials exist with unprecedentedly large dielectric constants reaching several thousands. The spontaneous polarization of a polar nematic material was found to be an order of magnitude higher [3] than that of classical ferroelectric liquid crystals, indicating extraordinary behaviour and strong interaction with electric fields. We studied RM734 that exhibits a ferroelectric nematic phase below a normal dielectric nematic phase. We investigated the behaviour of droplets of RM734 exposed to electric fields provided by in-plane and between plates electrodes. We found distinct regimes of electric-field induced spreading with various unusual morphologies (Fig.1a), depending on the temperature and the electric field. We find extraordinary electric field induced wetting and spreading properties of RM734 compared to conventional nematic and isotropic fluids.
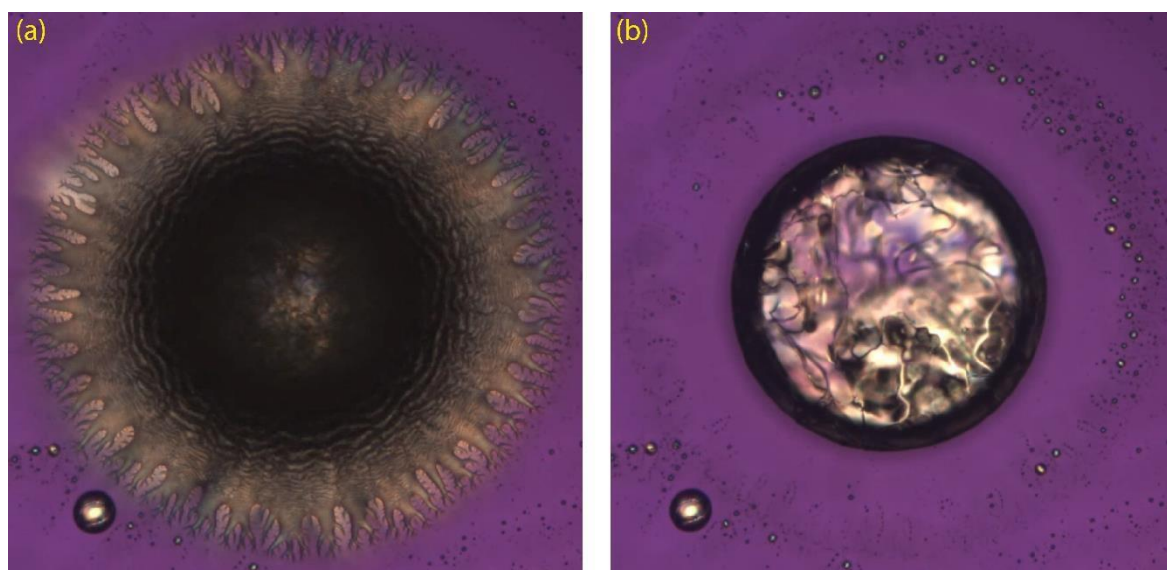

Figure 1: Unusual electric-field-induced spreading morphology (a), recovered droplet after switching the voltage off (b).

[1] H. Nishikawa, K. Shiroshita, H. Higuchi, Y. Okumura, Y. Haseba, S. Yamamoto, K. Sago, H. Kikuchi, Adv. Mater. **29**, 1702354 (2017)
[2] A. Mertelj, L. Cmok, N. Sebastián, R.J. Mandle, R.R. Parker, A.C. Whitwood, J.W. Goodby, M. Čopič, Phys. Rev. X **8**, 041025 (2018)
[3] X. Chen, E. Korblova, D. Dong, X. Wei, R. Shao, L. Radzihovsky, M. A. Glaser, J.E. Maclennan, D. Bedrov, D. M. Walba, N.A. Clark, PNAS **117**, 14021 (2020)

Dielectric and polar properties of the ferroelectric nematic phase.

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The recent discovery of ferroelectric nematic phases [1-4] represents a major development in liquid crystal research with deep implications in both fundamental and applied science. The large values of the dielectric constants ($>10^5$) and spontaneous polarizations of $\sim$ 6 $\mu C/cm^2$ reported ask for detailed and systematic studies of the dielectric and polar properties of such materials.

In this contribution, we present a thorough broadband dielectric spectroscopy study of RM734 in the 10^{-1}-10^8 Hz range, which shows pretransitional effects and a complex behavior in the ferroelectric phase. Results in the nematic phase are compared with those of an analogous material exhibiting only the classical nematic phase. Finally, we have also performed an in-deep analysis of spontaneous polarization measurements that evinced flow induced effects
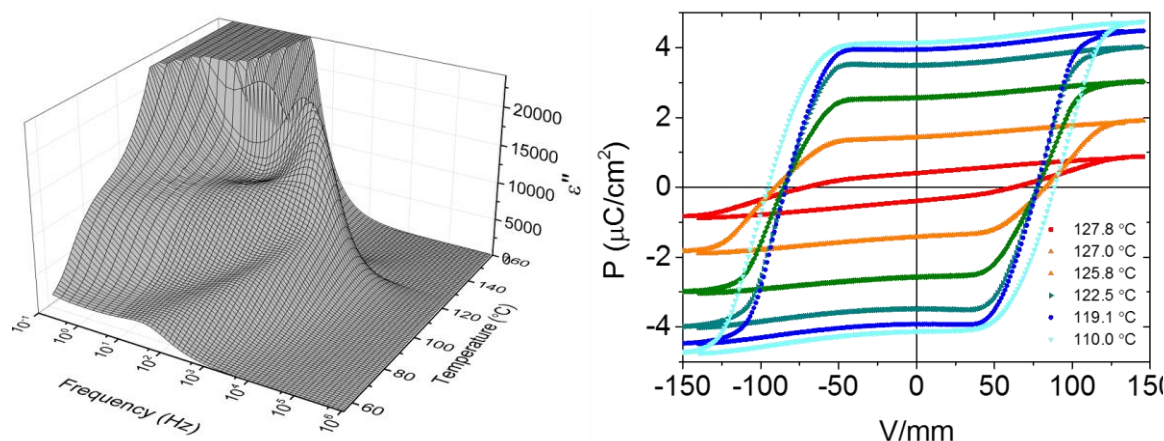

Figure 1: Left: 3D plot of the imaginary part of the electric permittivity of RM734 showing the nematic and ferroelectric phases in the anaylized frequency range. Right: Polarization hysteresis plots at several temperatures.

[1] A. Mertelj, L. Cmok, N. Sebastián, R. J. Mandle, R. R. Parker, A. C. Whitwood, J. W. Goodby and M. Čopič, Physical Review X, **8**, 041025 (2018).
[2] N. Sebastián, L. Cmok, R. J. Mandle, M. R. de la Fuente, I. Drevenšek Olenik, M. Čopič and A. Mertelj, Phys. Rev. Lett., **124**, 037801 (2020).
[3] R. J. Mandle, N. Sebastián, J. Martinez-Perdiguero and A. Mertelj, Nat. Commun. **12**, 4962 (2021).
[4] X. Chen, E. Korblova, D. Dong, X. Wei, R. Shao, L. Radzihovsky, M. A. Glaser, J. E. Maclennan, D. Bedrov, D. M. Walba and N. A. Clark, Proc Natl Acad Sci USA, **117** (25) 14021-14031 (2020).

Optimization of liquid crystal anchoring induced by polymeric ribbons with surface relief gratings

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Several characteristics of LC devices are determined by the LC surface alignment at the interfaces with the confining structures. As the fabrication techniques advance, more and more sophisticated alignment configurations can be designed and created. We report on the investigation of the effect of ITO film on the LC azimuthal anchoring energy in the compartmentalized microstructures obtained by sparse out-of-plane polymeric ribbons [1]. The ribbons with surface relief gratings on their sidewalls are fabricated by the two-photon polymerization-based direct laser writing (TPP-DLW) method. We found that the presence of ITO film on the glass substrates influences the azimuthal anchoring energy of the microstructures. This happens because the reflectivity of the ITO film can strengthen the standing wave formation taking place during the TPP-DLW process, which consequently affects the generation of surface gratings. An ITO film with a certain thickness that induces the highest light reflectivity results in an increased modulation depth of the surface undulation, thereby enhancing the anchoring energy for the LC molecules. By optical polarization microscopy of the LC cells prepared with the ribbon structures fabricated at optimal conditions, we show that, when the distance between the adjacent ribbons of the pattern is small enough, the resulting design promotes a very homogeneous and strong planar anchoring of the LC molecules.
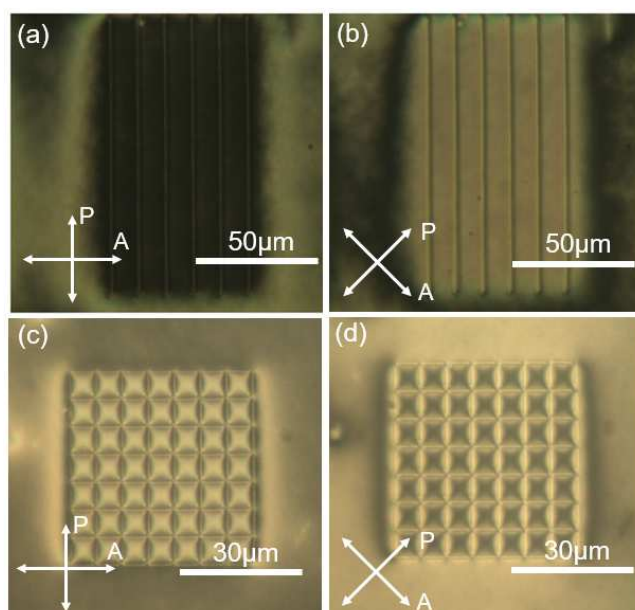

Figure 1. Polarization optical microscopy (POM) images of the nematic LC mixture E7 filled into one-dimensional (a, b) and two-dimensional (c, d) polymeric microstructures fabricated at optimal conditions for obtaining strong surface anchoring at the polymer sidewalls. White lines indicate transmission directions of the polarizer (P) and the analyzer (A). The images reveal a very good LC alignment inside the regions of the polymer scaffold structures, while outside that region, an unaligned LC texture is observed.

[1] Z. Ji et al., *Opt. Lett.*, **41**, 336 (2016).

Cross-differential dynamic microscopy: A tool for studying wavevector-dependent dynamics in soft matter

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We demonstrate the use of a dual-camera-equipped microscope for the study of the wavevector-dependent dynamics of soft matter. Contrary to the standard differential dynamic microscopy (DDM), in which a series of digital video images is acquired with a single camera at a constant frame rate, we use two randomly triggered cameras to obtain two sequences of images of the same region in the sample. We show how a weighted normalization technique decreases noise in the acquired cross-correlation function. We show that this technique can significantly reduce the time delay, which allows us to measure high-speed dynamics that could not have been performed with a single camera setup. We demonstrate the technique by studying flow-driven Brownian motion and wavevector-dependent director fluctuations in nematics. The method is robust, easy to implement, and a valuable tool for scientists studying the dynamics of colloidal systems, liquid crystals, liquid interfaces, etc.
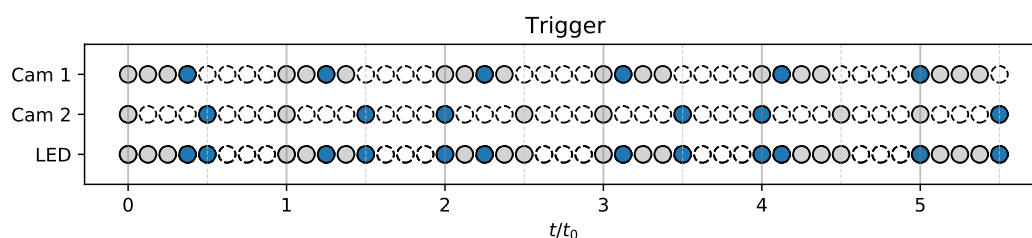
Figure 1: We select trigger times (blue circles) for the two cameras and the light source from a set of allowed times (gray circles). In the example above, $t_0 = 8$ time steps. Using standard (low FPS) cameras, the triggering scheme allows us to obtain short lag times with low data throughput.

[1] Soft Matter, 2019,**15, 2791-2797**

The improved synthetic method towards highly polar cyano and nitro terminated diesters

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Highly polar nematics with positive dielectric anisotropy are valuable components of many types of liquid crystalline materials. Starting from conventional positive nematics to nematics with dual frequency functionality or recently discovered splay nematic phase[1]. From many years ester derivatives of 4-cyanophenols or with other polar terminal substituent were known from generation of large longitudal dipole moment[2]. To extend the molecular core and further increase the parallel component of dipole moment, the second ester group have been often employed[2], [3]. Laterally nonsubstituted compounds of that type suffers from high melting points, additionally combination of two ester linkages and presence of cyano or nitro group limits the possible synthetic approaches. In our studies, we were focused on solving the high melting points and synthetic inconveniences of known cyanodiesters and nitrodiesters and present the synthesis and basic properties of materials with general structure presented below.
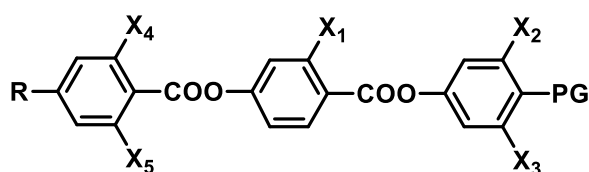
where

PG - Polar Group CN or NO_2
R - alkyl or alkoxy
X_1 to X_5 - F or H or alkoxy group

Fig.1 General structure of synthesized compounds.

[1] A. Mertelj *et al.*, "Splay Nematic Phase," *Phys. Rev. X*, vol. 8, no. 4, p. 041025, Nov. 2018, doi: 10.1103/PhysRevX.8.041025.

[2] H. Xianyu, Y. Zhao, S. Gauza, X. Liang, and S.-T. Wu, "High performance dual frequency liquid crystal compounds," *Liq. Cryst.*, vol. 35, no. 9, pp. 1129–1135, Sep. 2008, doi: 10.1080/02678290802389589.

[3] J. Czub, R. Dąbrowski, S. Urban, and D. Ziobro, "Dielectric properties of strongly polar nematogens," *Zeitschrift fur Naturforsch. - Sect. A J. Phys. Sci.*, vol. 65, no. 3, pp. 221–230, 2010, doi: 10.1515/zna-2010-0311.

Design and synthesis of photosensitive bent-core liquid crystals

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Contemporary research of liquid crystals (LCs), unique substances representing important materials of the current information age, is mainly focused on advanced self-assembling systems. Among them photosensitive materials play a prominent role due to broad applications in non-linear optics and photonics. From the variety of photosensitive units, the azo group stands out for its chemical stability and the distinct conditions of photoisomerization of the thermodynamically more stable *E*-(*trans*-)isomer to the photochemically preferred *Z*-(*cis*-)isomer and *vice versa*. Hereby, we introduce new photosensitive bent-core LCs based on previously established central units, namely 3-hydroxybenzoic acid [1,2]. With the aim to tune their mesomorphic properties, the type of the linking unit in the lengthening arms has been varied with increasing rigidity from benzoate ester and biphenyl to azo moieties. The properties of the materials have been further tuned by the lateral substitution (F, Cl) in the position 4 of the 3-hydroxybenzoic acid core, and the length of terminal alkyl chains (**Figure 1**). The effect of the reversal of one ester linkage on the mesomorphic behaviour was also investigated.

The structures of all materials and their intermediates were confirmed by ^{1}H and ^{13}C NMR spectroscopy. The mesomorphic properties of the studied materials have been determined from DSC, POM studies, and electro-optical investigation. The photoresponse of the new bent-core LCs was studied in solution as well as in the bulk mesophase.
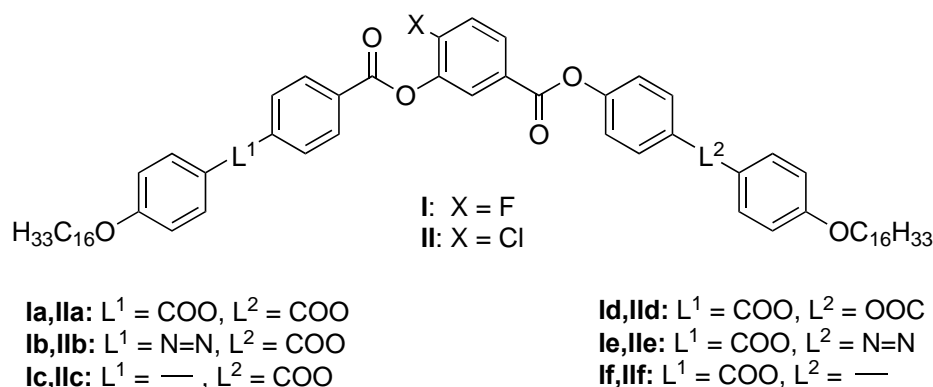

I: X = F
II: X = Cl

Ia,IIa: L^1 = COO, L^2 = COO
Ib,IIb: L^1 = N=N, L^2 = COO
Ic,IIc: L^1 = — , L^2 = COO

Id,IId: L^1 = COO, L^2 = OOC
Ie,IIe: L^1 = COO, L^2 = N=N
If,IIf: L^1 = COO, L^2 = —

Figure 1: The general structure of the studied materials

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Preparation of photosensitive axially chiral dopants for efficient amplification of chirality in liquid crystalline matrices

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Chirality is a highly fascinating phenomenon essentially connected with many fields of modern science such as chemistry, biology, physics, and related areas. We focus on preparation of novel chiral composites based on combination of achiral liquid crystalline (LC) matrices and axially chiral dopants. Resulting mixtures exhibit chiral mesophases that have attracted considerable attention due to their unique helical structure, which can be driven by external stimuli such as temperature, pressure or electric field. It predetermines them for many applications, *e.g.*, in non-linear optics, issue thermometers or organic compounds sensors. Amplification of long-range chiral order in the achiral matrix [1] has many advantages in comparison with preparation of optically pure mesogens. Specifically, this approach can solve some problems related with synthesis of chiral liquid crystals (racemisation, difficult purification and high costs). Moreover, combination of different types of matrices, dopants and their ratios is versatile and offers high variability of final materials and possibility how to easily enhance their properties.

We introduce new series of photosensitive axially chiral dopants based on the (*S*)-1,1'-binaphtalene core with various substituents. Binaphtalene derivatives are ideal candidates especially for their high helical twisting power (HTP) and stability. Due to photosensitive azo linkages directly connected to the chiral core (Fig.1a)), it is possible to change the properties of developed chiral superstructures dynamically by external light source (Fig. 1b)) [2]. Based on this investigation, we intend to use the best performing materials for preparation of ligands for decorating magnetic nanoparticles in future research thereby introducing an additional functionality into liquid-crystalline composites.
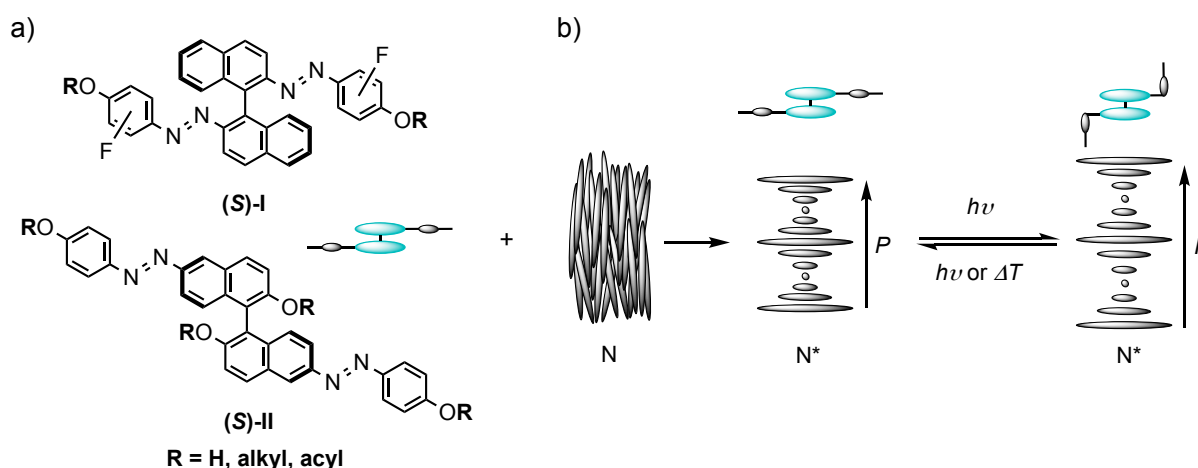

Figure 1: a) General structure of prepared dopants b) amplification of chirality and phototuning of the helical structure.

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Investigation of the tilt angle and spontaneous polarisation of antiferroelectric liquid crystals with a chiral centre based on (S)-(+)-3-octanol

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The antiferroelectric liquid crystals with molecular tilt nearly 45° are termed as orthoconic antiferroelectric LCs (OAFLCs) since angle between molecules in two neighboring layers is 90° [1, 2]. We focused on this group of materials because OAFLCs provide the switching times as fast as the conventional antiferroelectric LCs, but combined with a potentially much higher optical contrast.

The eight chiral smectic liquid crystals (SLCs) - [(S)-4'-(1-ethylhexyloxycarbonyl)biphenyl-4-yl 4-[n-(2,2,3,3,4,4,4-heptafluorobutoxy)alkyl-1-oxy]benzoates] were synthesised and tested. These compounds have the acronym: II.n.(X$_1$X$_2$) (S), where n=3-7; X$_1$, X$_2$= H or F. The electro-optical properties (tilt angle of the director and spontaneous polarisation) of the compounds were measured, see Figure 1.
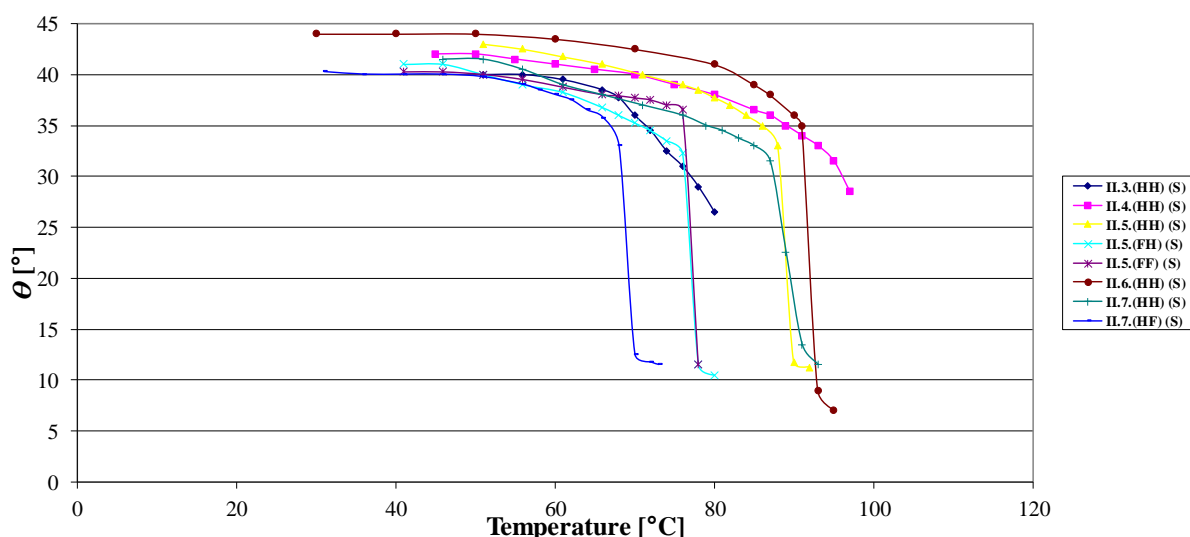

Figure 1. Temperature dependence of the tilt angle for all SLCs.

The compounds possess the self-assembling behaviour with an antiferroelectric ordering in smectic C$_a$* phase at a broad temperature range, some of materials have also a ferroelectric smectic C* phase and/or an orthogonal smectic A* phase. Due to high chemical stability and very high values of the optical tilt angle (40-44º) at saturation, the tested compounds can be used as chiral components for the orthoconic antiferroelectric liquid crystalline mixtures. The helical pitch for the compounds and formulated mixtures was also measured and discussed.

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Mirror symmetry breaking in achiral polycatenars with thioalkyl tails

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Mirror symmetry breaking in systems composed of achiral molecules is of importance for the design of functional materials as well as for the understanding of the mechanisms of emergence of prebiotic chirality.[1-3] Herein, we report the liquid crystalline behaviour of new rod-like achiral polycatenar molecules derived from π-conjugated 5,5'-diphenyl-2,2'-bithiophene core with a fork-like triple alkoxy chain at one end and a variable thioalkyl chain at the other end (Figure 1). It was found that helical self-assembly of the π-conjugated rods in networks takes place, leading to the appearance of a racemic ($Ia\overline{3}d$, gyroid) bicontinuous cubic phase for the shortest homologues which is replaced upon chain elongation by a spontaneous mirror symmetry broken ($I23$) bicontinuous cubic phase and a chiral isotropic liquid phase ($Iso_1^{[*]}$). Further chain elongation removes the $I23$ phase and replace it with the $Ia\overline{3}d$ phase again, indicating the presence of two different types of gyroid bicontinuous cubic phases with different pitch lengths. For some compounds additional 3D non-cubic tetragonal phase was observed as intermediate phase between the cubic $Ia\overline{3}d$ and $I23$ phases. The cubic phases exist over a wide temperature range and even at ambient temperatures for some derivatives. The reported materials could be of interest for the application as templates for chiral recognition and enantioselective catalysis.
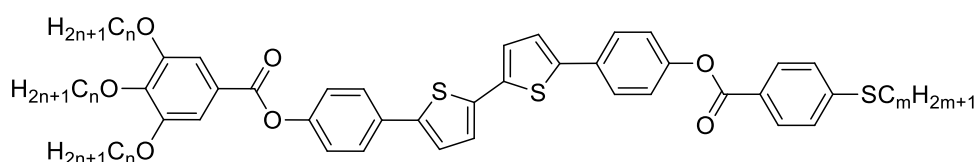

Figure 1: Chemical structure for the compounds under discussion.

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Indirect Measurement of the Electrocaloric Effect Close to the Ferroelectric Phase Transition in Ferroelectric Liquid Crystals

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Refrigeration technology based on the vapour-compression cycle has revolutionised society, but it has limitations, especially its use of greenhouse gases as refrigerants, the inability to miniaturise, and its slow start-up speed. Therefore, there is a growing demand for alternative cooling technologies that overcome these issues, and one possible technology could be based on using the electrocaloric effect (ECE) – reversible temperature change induced by adiabatic entropy change in the material, in response to rapid variation in electric field strength.

Since the revival of the topic thanks to the prediction of a large temperature change of 12K [1], research has focussed on solid state ferroelectrics. However, there are still engineering challenges around moving heat between the heat source and sink cyclically. A possible solution is to use dielectric liquids, such as liquid crystals, to make a system analogous to vapour-compression refrigeration. Before a cooling system can be made though, an extensive study on the ECE in liquid crystals is required to understand whether the magnitude of temperature change, available in the different possible liquid crystal systems, would be compatible with applications.

In this study, the ECE in various ferroelectric liquid systems was measured to understand the potential of a liquid crystalline analogy to solid ferroelectric materials. The spontaneous polarisation was measured using the current reversal method, and DSC was used to measure the volumetric heat capacity. With these values, indirect measurements of the electrocaloric temperature change can be made around the transition temperature into the ferroelectric phase. The results are discussed with respect to both material and device parameters.

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Effects of heliconical cholesteric LCs on light polarization

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Heliconical cholesteric liquid crystals are a recently proposed novel class of liquid crystalline materials that allow an efficient tuning of the chiral pitch through an external electric field parallel to the helix axis [1,2]. In this contribution we aim at studying an additional property of heliconical liquid crystals, that is their rotatory power and its dependence on an external field. To this purpose we performed a detailed study of the polarization of light propagating through a heliconical cholesteric cell when the LC pitch is tuned in a neighborhood of the resonance wavelength. Pitch tuning is obtained by applying to the cell an external electric field or with the aid of an optical field in a pump-probe configuration [3,4]. Results show that linearly polarized light undergoes optical rotation in the neighborhood of the resonant pitch and becomes nearly circularly polarized when the pitch meets the resonant value at electric field $E_R = 2.75\,V/\mu m$ or equivalently at pump intensity $I_R = 12.71\,kW/cm^2$ (Figure - first two rows).
. Circularly polarized light is instead totally reflected or transmitted depending on the handedness, keeping its original polarization state. (Figure - last two rows)
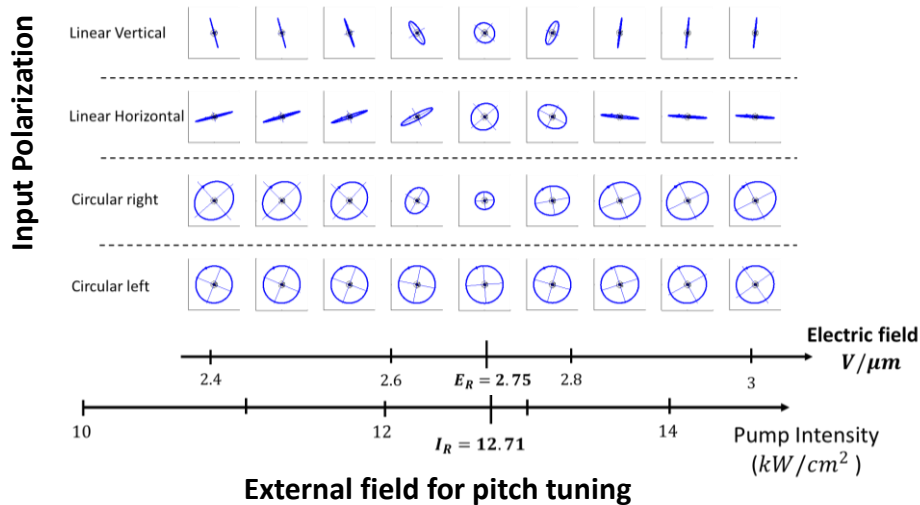

Figure 1: Effect of electric field on the polarization of light propagating trough an heliconal cholesteric liquid cristal

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Spectral properties of photonic crystal fibres infiltrated with titanium dioxide nanoparticles-doped ferroelectric liquid crystals

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Photonic liquid crystal fibres (PLCFs) have attracted significant attention of many research groups since the beginning of the XXI century due to their electro-optical properties. The PLCFs can find many practical applications, including tuneable long-period fibre gratings [1], attenuators [2] or polarization controllers [3]. The innovative in-fibre optical devices require liquid crystals (LCs) with improved properties. Chiral smectic C (SmC*) LCs, also called ferroelectric liquid crystals (FLCs), are especially attractive for this purpose mainly due to their fast electro-optical response at low electric fields. It has been observed that the application of aligning materials to FLCs [4] and doping of nanoparticles in FLCs [5] can further enhance their electro-optical parameters like faster switching times, lower operating voltages, and luminescent properties.

In the present study, we have focused on investigations of spectral properties of isotropic PCFs infiltrated with two FLC mixtures doped with titanium dioxide (TiO_2) NPs in different concentrations. As a host material, we have used an LMA-10 isotropic PCF in which we have generated an aligning surface to improve the orientation of the NP-FLC nanocomposite molecules along the PCF's air holes. Two types of FLC mixtures were considered in our studies, a W212 FLC and W206 FLC (both with different values of the spontaneous polarization) in which TiO_2 NPs were dispersed. We have analysed the influence of NPs concentrations on response times of the investigated PLCFs under the influence of the external electric field.

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Liquid Crystalline Phases of DNA-Quadruplexes from d(G_4C_2) and d(G_4C_2)$_2$ Sequences

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Guanine-rich DNA sequences self-assemble into fourfold helical structures called DNA-quadruplexes. End-to-end stacking of these quadruplexes causes the formation of long rodlike aggregates that can, at higher concentrations, exhibit a lyotropic liquid crystalline (LC) behaviour. The pioneering work of Gottarelli *et al.* showed that self-assembled single guanosine molecules had a rich LC polymorphism [1]. Later, LC phases of DNA molecules and short oligonucleotides were intensively studied [2,3]. Up to date, however, much less is known about the LC behaviour of DNA-quadruplexes in concentrated solutions.

We studied LC formation of DNA sequences G_4C_2 and $(G_4C_2)_2$. The $(G_4C_2)_n$ sequences are associated with some fatal neurological disorders, especially amyotrophic lateral sclerosis (ALS) and frontotemporal dementia (FTD). We previously confirmed, by dynamic light scattering and atomic force microscopy, that both investigated sequences formed G-quadruplexes, with G_4C_2 forming extremely long ($L > 50$ nm) 1D aggregates (G-wires) [4].

For this work, we prepared highly concentrated ($c > 50$ mM) aqueous solutions of G_4C_2 and $(G_4C_2)_2$ that were incorporated into thin glass cells and imaged by polarization optical microscopy (POM). Both sequences showed LC behaviour, with the G_4C_2 showing columnar LC phases (Fig. 1) similar to those observed for short DNA duplexes [2], while $(G_4C_2)_2$, in contrast, exhibited a surprising monotonic anisotropic texture.
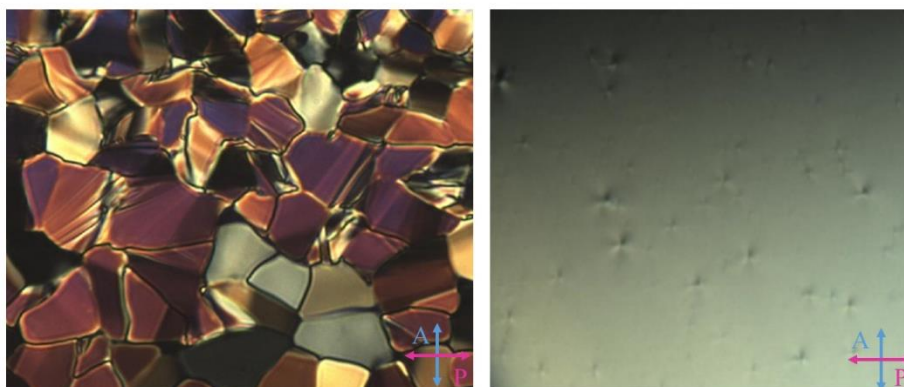

Figure 1: Lyotropic liquid crystal phases of DNA sequences G_4C_2 (left) and $(G_4C_2)_2$ (right).

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Defects induced by anchoring transitions of nematic fluids at solid and gas interfaces

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In nematic liquid crystals, the average molecular orientation, the director is usually considered fixed at a surface. Nevertheless, rarely in some specific combinations of the liquid crystal and the bounding material, one can observe a so-called anchoring transition, which is a continuous or discontinuous change in the director at the surface depending on the temperature. In our investigations, one aim was to find nematic liquid crystals that undergo a temperature induced anchoring transition on the specific perfluoropolymer surface CYTOP in order to broaden the range of materials that exhibit a discontinuous anchoring transition [1]. We established a searching algorithm based on sessile droplets (see Figure 1) allowing an efficient discovery of compounds that show anchoring transitions not only at CYTOP surfaces but at interfaces with air as well. As a result, we identified new compounds that show anchoring transitions either on the CYTOP coated substrate or at free surfaces bounded by air. As a consequence of the two types of anchoring transitions, we revealed two distinct textural transitions in spherical caps of NLCs governed by the reorganization of the director field and the appearance of different types of defects. In order to understand such anchoring transition induced restructuring of the director field, we performed optical simulations of the sessile droplets.
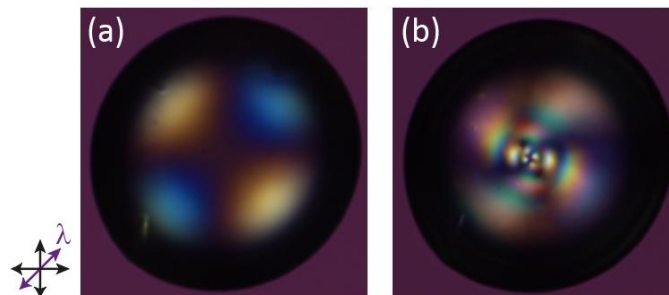

Figure 1: Typical textures of sessile droplets with homeotropic (a) and radial planar (b) boundary conditions at the supporting flat surface (with homeotropic alignment at the air interface).

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Polarization rotation by cholesteric layers with tangential-conical boundary conditions

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Cholesteric liquid crystal (CLC) is a chiral molecular system with high sensitivity to external factors. Nowadays, the CLC cells with tangential, homeotropic, and hybrid homeplanar boundary conditions are well studied. Recently, the orientational structures of CLC with tangential-conical boundary conditions have been investigated [1,2]. In the present work, we consider the polarization characteristics of light passed through such CLC cells.

The experiment was carried out with sandwich-like cells consisting of two glass substrates coated with polymer films and the cholesteric layers of various thickness between them. The nematic mixture LN-396 (Belarusian State Technological University) doped with the left-handed chiral additive cholesterylacetate was used as a cholesteric liquid crystal. One substrate was covered by the polyvinyl alcohol and another one was covered by poly(isobutyl methacrylate) which for LN-396 specify the tangential and conical boundary conditions, respectively. The ratio of CLC layer thickness d to the helix pitch p was 0.61 for all samples under study.
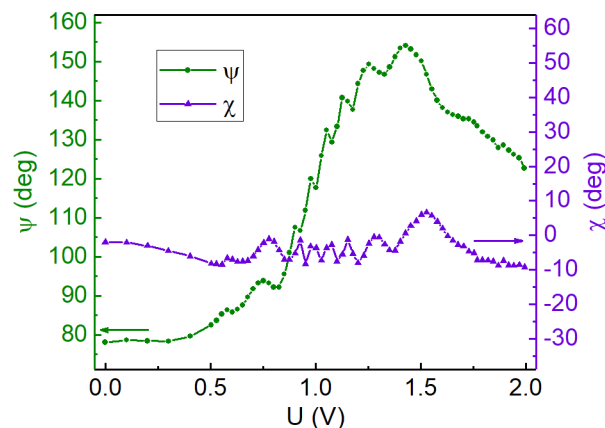

Figure 1: Experimental dependence of the polarization azimuth ψ and ellipticity angle χ of the transmitted light from the applied voltage U. Thickness of CLC layer $d = 35.3$ μm. Cholesteric pitch $p = 57.6$ μm. Wavelength of incident linear-polarized light $\lambda = 632.8$ nm.

It has been revealed that considered CLC cells with tangential-conical boundary conditions can operate as electrically controlled achromatic polarization rotator. Such cells allow turning the polarization azimuth more than 70° using the control voltage less than 2 V. The observed behaviour of polarization rotation is connected with the unique untwisting effect of the cholesteric helix due to the free azimuthal rotation of the director on the substrate with conical anchoring.

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Simple and time-saving transfer matrix method for analysis of light propagation in helically twisted liquid crystals

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In the recent years, helically twisted (chiral) nano- and micro-structures have risen widespread attention in the field of optics as promising materials for light field regulation, optical sensing, optical communications, and construction of various new types of optical devices. Therefore, it became an important challenge to develop computational procedures that enable fast and accurate analysis of propagation of optical radiation through such structures. Cholesteric liquid crystals (CLCs) are natural examples of periodic helically twisted optical media. They have many intriguing properties and are also interesting as nonlinear optical materials. Due to their strong response to various external stimuli, CLCs were found to be very suitable for construction of wavelength tunable lasers and laser displays [1-3] that provide an efficient control of light propagation modes and are low cost and quite simple to be fabricated. According to the model proposed by Chandrasekhar and Srinivasa Rao [4], and by Nityananda [5], CLCs can be regarded as a stack of thin optically uniaxial layers with a very small twist angle between the neighboring layers. Based on this model, we developed a general transfer matrix formalism for helically twisted layered structures. The evolution of optical electric field for the optical wave propagating along the helical axis is calculated on the basis of circularly polarized and on the basis of linearly polarized components. The transmission and reflection spectra are deduced. The corresponding computational method is very simple and time saving and suitable for exploration of any kind of twisted liquid crystal configuration.

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Diffraction of light at oblique helicoidal cholesteric

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Chiral nematics with a small bend elastic constant form an oblique helicoidal cholesteric (Ch_{OH}) in an external electric field [1-2]. Both the period P and the cone angle θ of Ch_{OH} are tunable by the applied field. The Ch_{OH} state forms in chiral mixtures containing flexible dimers with bent conformations. At the normal incidence of light, reflection from the Ch_{OH} half-pitch $P/2$ is electrically tunable in a broad spectral range, including the visible part. At the oblique incidence of light, two periodicities associated with the full P and the half-pitch $P/2$ are observed in reflection, both tunable by the electric field E and the angle of incidence β, Fig.2. The full pitch P bandgap is characterized by a wide bandwidth and total reflection at a large angle of oblique incidence. When the incident light is linearly polarized, a linear polarization perpendicular to that of the incident light is reflected by the full pitch P, Fig.2(a). The half-pitch $P/2$ bandgap shows red and blue shifted spectra for p- and s-polarized light, respectively, with the central spectral region of the bandgap having similar polarization characteristics as the full pitch, Fig.2(b). The work is supported by the NSF grant ECCS-1906104.
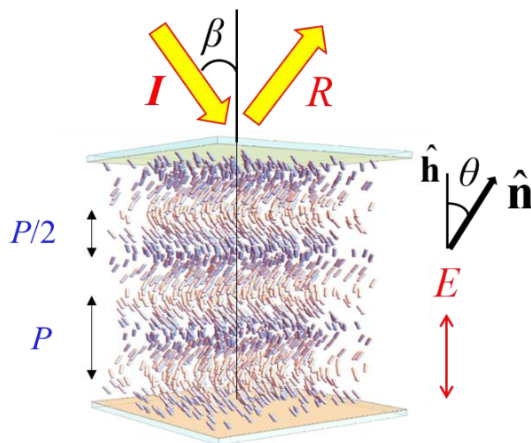

Fig. 1. Oblique helicoidal cholesteric structure with the pitch P and the cone angle θ tunable by applied electric field **E**. At the oblique incidence of light, two periodicities associated with the full P and the half-pitch $P/2$ are observed in reflection. Notation for angles: β is the angle of incidence, θ is the cone angle.
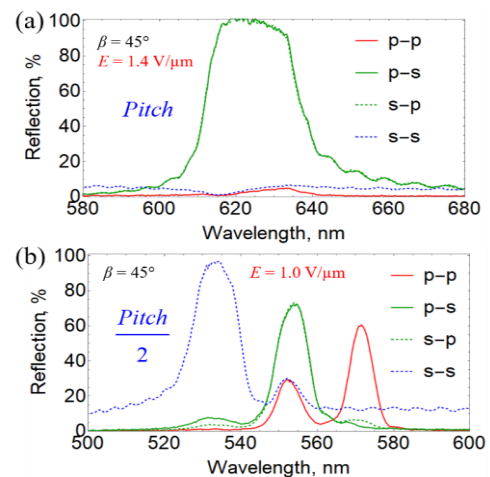
Fig. 2. Polarization characteristics of reflection from (a) the full P and (b) the half-pitch $P/2$ in the planar Ch_{OH} cell, $d = 23$ μm, at the angle of incidence of polarized light $\beta = 45°$.

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Supramolecular chiral N_{tb} phase in symmetric dimers - α,ω-bis(4'-cyano-3'-fluorobiphenyl-4-yl)alkanes

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Undoubtedly, the experimental confirmation of the existence of the nematic twist-bend N_{tb} and nematic splay N_s phase are the most significant discoveries in the last few years in the field of liquid crystals [1,2]. The supramolecular chiral structure composed of achiral building elements is a characteristic feature of the N_{tb} phase, in which the average direction of the molecules changes by rotation around the axis of the helix and is additionally tilted by the same angle. The resulting structure can be clockwise or counterclockwise with nanoscale periodicity. The number of known compounds having a twist-bend nematic phase is small, mostly dimers of calamitic liquid crystalline compounds linked by a flexible aliphatic chain [3], but also trimers and tetramers [4]. A necessary condition for the induction of the N_{tb} phase is a non-linear, bent structure of the molecule, which is ensured by a methylene linker with an odd number of carbon atoms and the presence of non-covalent bonds between the conjugated aromatic ring systems of adjacent molecules. There is still no answer how the elements of the molecule structure affect the presence of the N_{tb} phase and its physicochemical properties, such as temperature range, viscosity, refractive indices or enthalpies of phase transition between phases. Observation is hindered, or even impossible, by the high temperature of occurrence of this phase, which limits the measurement capabilities of most of the available instruments.

In this work, new compounds from a homologous series of α, ω-bis (4'-cyano-3'-fluorobiphenyl-4-yl), α, ω-bis (4'-cyano-2-fluorobiphenyl-4-yl), α, ω-bis (4'-isothiocyanatobiphenyl-4-yl) and α, ω-bis (4'-trifluoromethoxybiphenyl-4-yl) alkanes have been synthesized and investigated. The temperatures and enthalpies of phase transitions have been designated for all obtained compounds, while dynamic viscosity, refractive indices and dielectric anisotropy have been examined for compounds exhibiting N_{tb} phase. The eutectic mixture having N_{tb} phase at room temperature has been developed. The presence of fluorine atom in lateral position to benzene ring lower the phase transition temperatures, both melting and clearing, thereby allowing to obtain a low temperature N_{tb} phase.
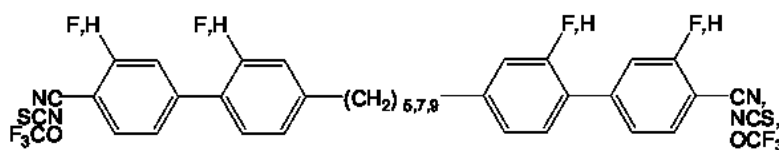

Figure 1: General molecular formula of the synthesized dimers.

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Twist-bend nematic phase: possible applications of periodic structures

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Twist-bend nematic phase (N_{TB}) has recently become one of the major attractors in Liquid Crystal (LC) research. A wide range of materials including mesogenic dimers and bend-core LCs have been reported to possess this phase. Stable presence in mixtures and availability at the room temperature make is ready for applications. However, the intrinsic complexity of this phase is currently the most intriguing property to be understood.
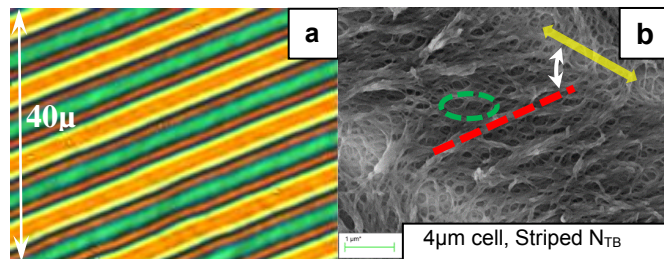

Figure 1: Structures in NTB phase: (a) Polarizing optical microscope image of 5µm thick planar cell [3], (b) Scanning electron microscope image of polymerized submicron structures [4].

Among other attractive properties of the N_{TB} phase, such as fast reaction to electric field and unusual values of elastic constants [1], is the ability to form periodic patterns. The phase forms a complex hierarchy [2] of structures ranging from sample-size stripes visible in optical microscope (Figure 1a), via submicron fish-bone (Figure 1b), to molecular-level helix with 8 nm pitch [5].

An overview of to-date findings and research methods will be presented. We will also report our most recent findings in using of the patterns to form specialized polarized beams for telecommunications.

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Ferroelectric nematics in microchannels: switching and propagation of order

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We produced, via laser ablation, microchannels buried in glass that connect gold electrodes, silanized their surfaces, and filled them with RM734, a liquid crystal material that exhibits nematic (N) and ferroelectric nematic (N_F) phases [1-3]. The channels are 1-2 mm long and 25 μm wide. Silanization favors planar orientation of RM734 [4], inducing nematic ordering along the axis of the channel. By applying electric fields as low as 1V/mm to the N_F phase, we observe a marked improve of the nematic ordering. Upon inverting the field, the nematic ordering becomes suddenly unstable, the channel transiently filling with defects, to later regain uniform alignment in a "soliton"-like feature, i.e. through the expansion of a defect free texture that nucleates where the channel is narrowest. Such propagation occurs in a time of the order of 10-100 ms that depends on the field strength.

We also considered highly bent channels, in which the continuity of the polar order along the channel axis could oppose the electric field direction, as in the picture. Also in this case, the N_F order develops continuously with no domain walls, suggesting that the electric field lines remain trapped within the N_F phase and follows the winding channels, in analogy with the bevavior of magnetic fields in ferromagnetic materials.
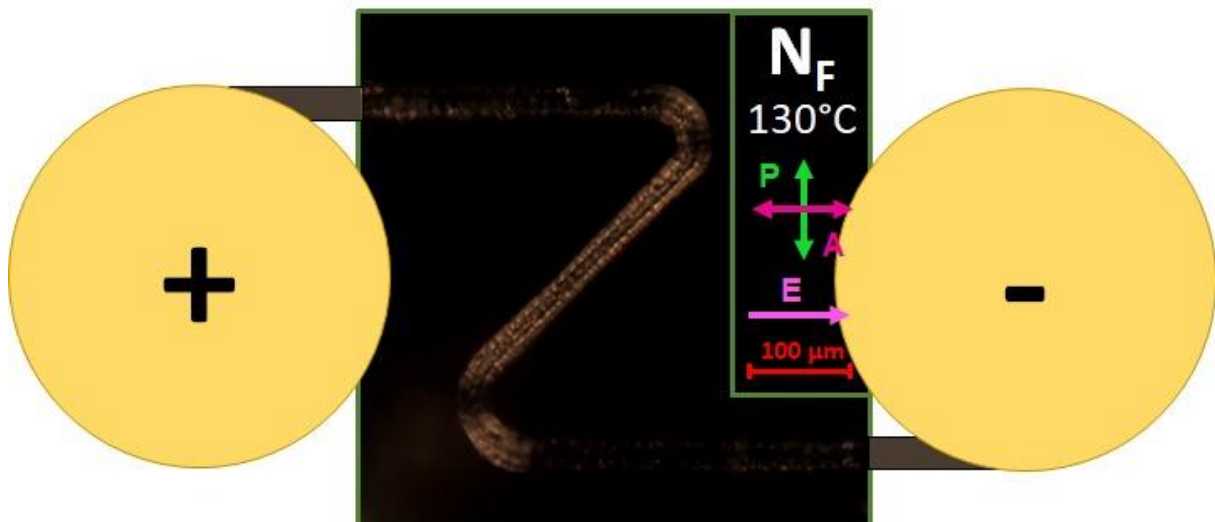

Figure 1: Polarized microscopy image of a "Z" shaped microchannel filled with RM734 during the appliance of a 1V/mm electric field through gold electrodes perpendicular to the channels, whose section is sketched in scale.

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Observations of bidirectional flow in ferromagnetic ferrofluids generated by uniaxial magnetic field

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We report observations of bidirectional flow in suspensions of magnetic nanoparticles in isotropic fluids under external alternating magnetic field. Magnetic nanoplatelets made from scandium-substituted barium hexaferrite [1,2], were dispersed in tert-butanol at concentrations forming ferromagnetic nematic phases. When placed in an external alternating magnetic field, we observed formation of bright and dark stripes under polarising microscope in the direction perpendicular to the magnetic field. Along the lines, which represent magnetic domains, fluid flow is observed. Most notably as transport of particles but also by performing space-time correlations of thermally excited fluctuations. We measured the velocity profile along the stripes and noticed that the velocity is the largest in black regions, reaching the values of several µm/s. Small angle neutron scattering has been used to help determine the origin of the observed flow.
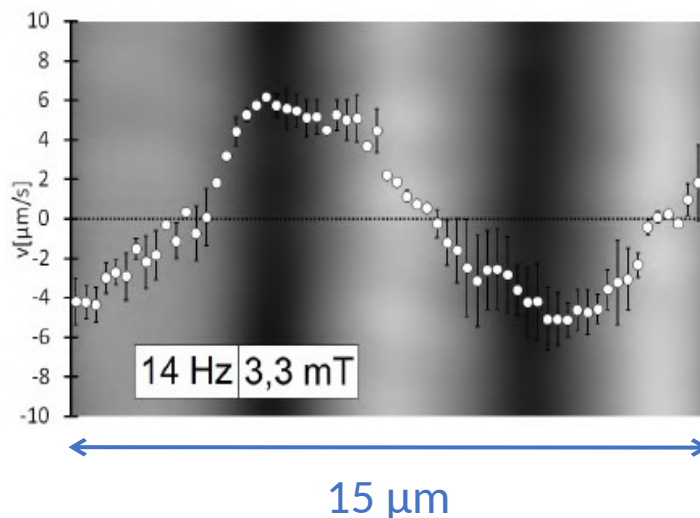
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Capillary flows of nematics and ferroelectric liquid crystals

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In this report, we present the results of comprehensive studies of capillary flows of nematic and ferroelectric smectic liquid crystal (FLC) C * in planar capillaries with a given surface orientation. The main goal of the experiments was to establish whether the theoretical models developed earlier for capillary flows of Newtonian fluids can be used to describe LC flows that generally demonstrate non-Newtonian behaviour. Experimental information was obtained by recording the motion of the contact line with a video camera and further processing the resulting images. In the case of a nematic, the capillary flow was satisfactorily described by the above models only when a strong electric field is applied, which stabilizes the orientational structure [1]. This made it possible to calculate the shear viscosity coefficient, which turned out to be close to Miesowicz viscosity.

At the same time, the capillary flow of a ferroelectric liquid crystal showed quasi-Newtonian behaviour in the absence of an electric field, which may be associated with the stabilizing effect of smectic layers.

The results obtained can be used to measure the anisotropic shear viscosity of liquid crystals.

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Electric Field and Light Induced Patterns in Hybrid Aligned Cholesterics

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The influence of light irradiation on electric field induced optical gratings was studied in two kinds of photosensitive liquid crystalline systems.

In system A , a cholesteric phase was induced by adding a photosensitive chiral dopant to a regular nematic host, yielding a UV-tunable helical pitch including the inversion of the helical sense. Application of an ac voltage induces electroconvection patterns. In planar samples, the orientation of the convection rolls can be switched via UV illumination between two orthogonal directions [1]. In hybrid aligned samples, however, the orientation of the voltage induced electroconvection rolls can be continuously and reversibly rotated by varying the intensity of the UV irradiation [2].

In system B, a photosensitive azo moiety was incorporated into the skeleton of a bent-core nematic. Irradiation by UV light induces a trans-to-cis photoisomerization, while illumination by blue light promotes cis-to-trans back relaxation. This substance exhibits flexoelectric domains upon applying a dc voltage. The threshold voltage of flexoelectric domains and thus their wavenumber too can be changed by light irradiation [3].

Both effects have a potential for light-switchable or continuously light tunable beam steering applications.

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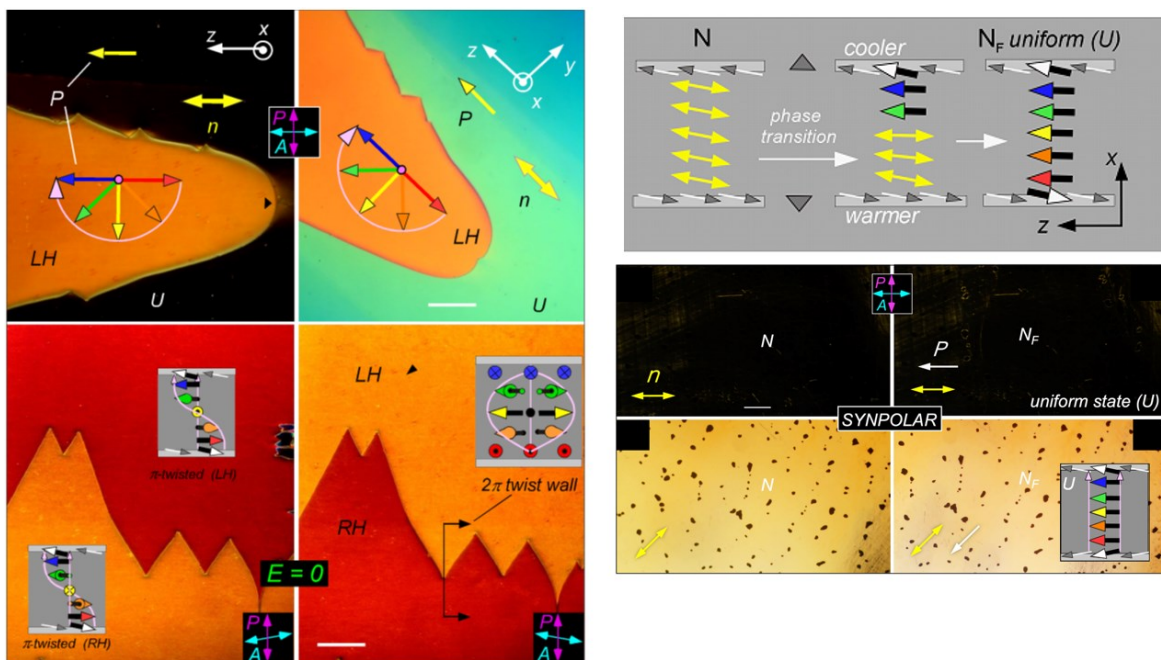[3] H. Jing, et al., Adv. Optical Mater. 7, 1801790 (2019),

Polar In-Plane Surface Orientation of a Ferroelectric Nematic Liquid Crystal: Polar Monodomains and Twisted State Electro-Optics

Xi Chen[1], Eva Korblova[2], Matthew A. Glaser[1], Joseph E. Maclennan[1], David M. Walba[2], Noel A. Clark[1]

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We show that surface interactions can vectorially structure the three-dimensional polarization field of a ferroelectric fluid [1]. The contact between a ferroelectric nematic liquid crystal and a surface with in-plane polarity generates a preferred in-plane orientation of the polarization field at that interface. This is a route to the formation of fluid or glassy monodomains of high polarization without the need for electric field poling. For example, unidirectional buffing of polyimide films on planar surfaces to give quadrupolar in-plane anisotropy also induces macroscopic in-plane polar order at the surfaces, enabling the formation of a variety of azimuthal polar director structures in the cell interior, including uniform and twisted states. In a π-twist cell, obtained with antiparallel, unidirectional buffing on opposing surfaces, we demonstrate three distinct modes of ferroelectric nematic electro-optic response: intrinsic, viscosity-limited, field-induced molecular reorientation; field-induced motion of domain walls separating twisted states of opposite chirality; and propagation of polarization reorientation solitons from the cell plates to the cell center upon field reversal. Chirally doped ferroelectric nematics in antiparallel-rubbed cells produce Grandjean textures of helical twist that can be unwound via field-induced polar surface reorientation transitions. Fields required are in the 3 V/mm range, indicating an in-plane polar anchoring energy of $W_P \sim 3\times10^3$ J/m^2.

Left: Uniform N$_F$ state in an antipolar cell (with antiparallel buffing) evolving spontaneously to a twisted configuration. Twist states of both handedness are observed. **Right**: Uniform polar state obtained in a synpolar cell (with parallel-buffed surfaces). Scale bars: 200 μm.

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The fourth fundamental mode of nematic director deformation: Delta mode

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A recent mathematical construction writes the Oseen-Frank free energy in terms of four fundamental deformation modes: splay, twist, bend, and the Delta mode [1,2]. Each of these modes is coupled to a specific type of molecular order: the twist mode with chirality, the bend and splay modes with polarization perpendicular and parallel to the nematic director, respectively, and the Delta mode with octupolar order [3]. If a liquid crystal has chiral order, it forms a cholesteric or blue phase with favored twist. Likewise, if it has polar order, it forms a twist-bend nematic, splay-bend nematic, splay nematic, or related modulated structure [4]. Based on this concept, we ask: What happens if a liquid crystal has octupolar order? To answer that question, we develop a Landau theory for octupolar order $\mathbf{\Omega}$ of extended tetrahedral molecules. We construct the free energy density in terms of the nematic director $\mathbf{n}$ and the octupolar order parameter,

$$
\begin{aligned}
F &= \frac{1}{2}(K_{11} - K_{24}) S^2 + \frac{1}{2}(K_{22} - K_{24}) T^2 + \frac{1}{2}K_{33}|\vec{\mathbf{B}}|^2 + K_{24}\operatorname{Tr}(\mathbf{\Delta} \cdot \mathbf{\Delta}) - \lambda\operatorname{Tr}(\mathbf{\Delta} \cdot \mathbf{\Omega}) \\
&+ \frac{1}{2}\mu\operatorname{Tr}(\mathbf{\Omega} \cdot \mathbf{\Omega}) + \frac{1}{4}\nu\operatorname{Tr}(\mathbf{\Omega} \cdot \mathbf{\Omega})^2 + \frac{1}{2}\kappa\,|\nabla\mathbf{\Omega}|^2.
\end{aligned}
$$

We study the structure of the modulated phases below the critical point. In particular, we show that the liquid crystal may form a cholesteric phase with either handedness, represented in Fig. 1(a), or a single-splay or double-splay state, shown in Figs. 1(b,c).
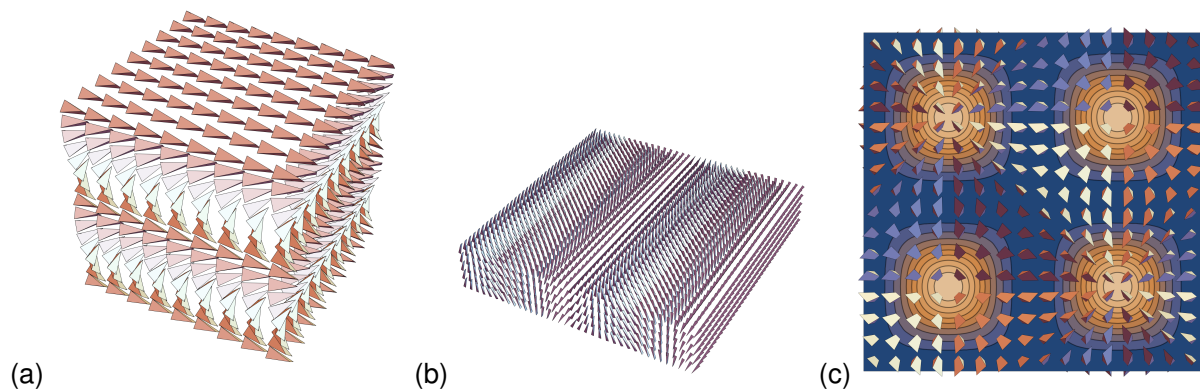

(a)　　　　　　　(b)　　　　　　　(c)

Figure 1: Schematic representations of proposed structures with extended tetrahedra in the nematic phase: (a) Cholesteric phase, (b-c) splay nematic phases with single and double splay, respectively.

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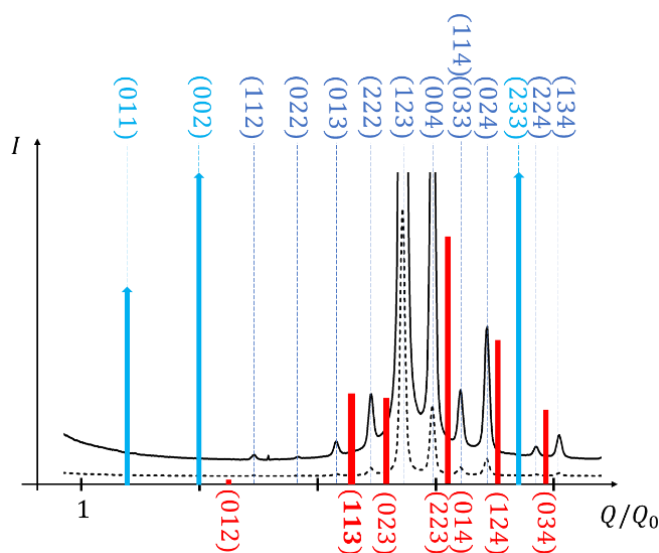# Modeling of the Resonant X-ray Response of a Chiral Cubic Phase

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Several structural models have so far been proposed for the structure of a continuous grid chiral cubic phase made of achiral constituent molecules, a phase, which is a hot topic in the field of thermotropic liquid crystals. Resonant X-ray scattering (RXS), gives information on the molecular orientation in the unit cell, and as such, it could help in selecting the most appropriate model. We modelled the RXS response [1] for the recently proposed structural model [2]. We constructed a tensor form factor of a unit cell and calculated intensities of the peaks for all Miller indices. We find that all the symmetry allowed peaks are resonantly enhanced and their intensity is much stronger than the intensity of the resonant peaks. We predict strong resonant enhancement of the symmetry allowed peaks (011) and (002) which are not observed in nonresonant scattering. These two peaks could be observed by RXS at the carbon absorption edge. By RXS at the sulphur absorption edge one might observe the resonant peak (113) and resonantly enhanced peak (233) plus resonant enhancement of all the peaks that are observed in a nonresonant scattering and which probably hide the rest of the predicted resonant peaks. The tensor form factor of another recent model of the chiral cubic phase [3] is currently under a construction and in our presentation we will compare the predicted RXS diffractograms for both models.

Figure 1: Intensities (in arbitrary units) of the diffracted peaks, measured by the nonresonant X-ray scattering (black curve) [2] and the predicted [1] resonant (red lines) and resonantly enhanced peaks (blue arrows) as a function of the normalised scattering vector magnitude (Q/Q_0), defined by the Miller indices (hkl).The intensities of the measured and calculated intensities cannot be compared.

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Engineering Optical Rotation in Chiral Photonic Film for Configurable Color Filter

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Photonic crystals (PC) are periodic optical micro- or nanostructures, and they have structural colors by reflecting a specific wavelength of light, also known as photonic bandgap (PBG)[1]. The structural colors are more stable than chemical dyes since they originate from light interference and are widely used in daily life. In chiral PC, there is optical rotation (β), in which the polarization axis of linearly polarized light rotates when it enters the chiral medium[2]. The optical rotation tends to diverge at PBG wavelength due to the photonic resonance effect and decrease in proportion to the square of the inverse of the wavelength at wavelengths much shorter than PBG region. The optical rotation dramatically varies depending on the wavelength of light, known as optical rotatory dispersion. It is the driving force for the color changes, and polarization-dependent color variation can be achieved by positioning the chiral PC film between two linear polarizers and rotating one polarizer[3].

Herein, we show polarization-dependent transmission color variation that depends on the optical rotation and PBG wavelength using cholesteric liquid crystals (CLC), which can act like 1D chiral PC by forming a spontaneous helical superstructure[4]. The PBG wavelength can be easily controlled by the concentration of chiral dopant. As a result, we can engineer PBG wavelength and optical rotation precisely, which enables the polarization-dependent color variation. The various colors can be expressed within one PC film by simply rotating the polarizer, and the color gamut is different depending on the position of the PBG wavelength. Moreover, when the PBG wavelength is located in IR range, this PC film can control the transmission of specific wavelength to 0% while remaining transparent. We developed an active type protective goggle using this characteristic, and various wavelengths are successfully blocked according to the rotation angle. We expect this polarization-dependent transmission color can open a new door in color variation technology.
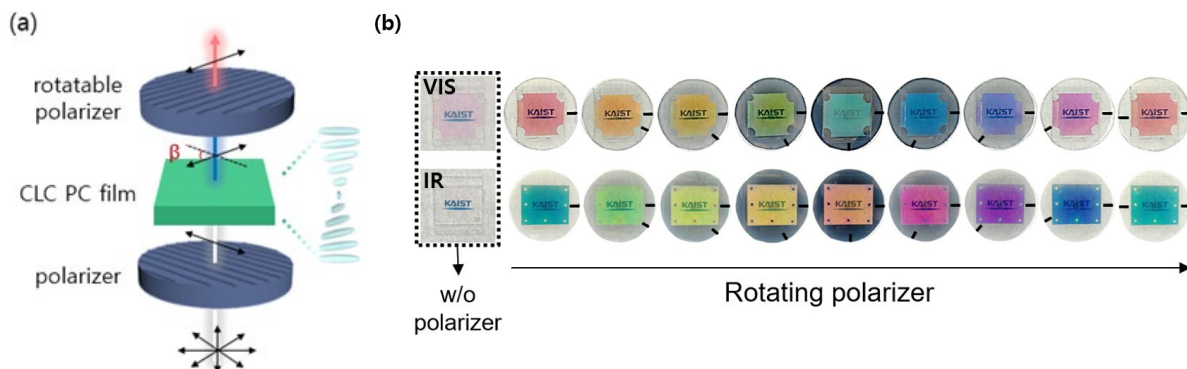

Figure 1: (a) Experimental set-up of transmission mode with two rotatable linear polarizers. (b) Polarization-dependent transmission color variation in chiral PC film.

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Design strategy of optical rotation for chiral liquid crystal-based optical application

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A chiral material can rotates the polarization state due to the phase difference between two circular polarization states of the transmitted light, which is called optical rotation. Many studies have been reported optical rotations in nature, such as quartz, sugar, and cholesteric liquid crystal (CLC) [1]. Especially, CLC has a photonic bandgap that resonantly reflects one CPL with the same chirality as the CLC layer by the periodic helical structure [2]. In addition, the geometric features of CLC can be manipulated by surface treatments and external stimuli. However, despite these advantages, optical applications based on the engineered optical rotation of CLC have not yet been demonstrated.

In this research, we introduce the strategy for the optical application with the rotated polarization state by the tailored supramolecular structure of CLC. The interaction between the CLC layer and linearly polarized incident light was simulated using the Berreman 4x4 method. In particular, where the wavelength of PBG is much longer than that of the incident light, CLC film is transparent, and its optical rotation is inversely proportional to the square of the wavelength. We propose a sandwiched CLC layer with one fixed polarizing film and one rotatable polarizing film as an analyzer to achieve an active color filter for the color-tunable laser goggle. Moreover, the goggle employing optical rotation engineered by manipulating the geometric features of CLC film can change the number and bandwidth of blocked wavelengths.
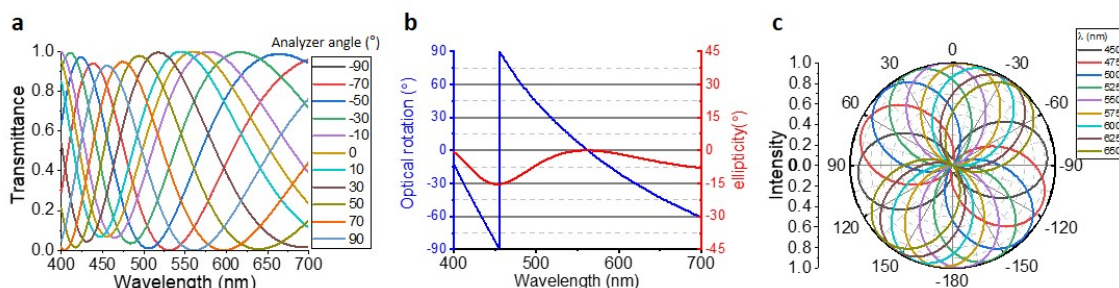

Figure 1: Calculated optical properties of CLC film of which pitch and birefringent refractive indices are $2.5 \mu m$, 1.6, and 1.7, respectively. a) Analyzer angle-dependent transmittance. b) optical rotation (blue) and ellipticity (red) of the transmitted light. c) the polarization state of the transmitted light depending on the incident wavelength.

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Numerical Modelling of Blue Phase III

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We report on a mesoscopic Landau de Gennes numerical modelling of blue phase III (BPIII) – an amorphous liquid crystalline phase made of entangled double-twisted cylinders (or skyrmions) and topological defect lines [1]. By changing the initial conditions of the sample, the liquid crystal relaxes to a number of different stable and metastable structures, which emerge in bulk and in constrained planar cell geometry. The amorphous BPIII structure is numerically stable and has the lowest total free energy in a narrow range of high temperature and high chirality, as shown in the calculated phase diagram. The numerical simulations provide insight into the detailed structures of these new materials, which correspond also to the experimental observation of the amorphous blue phase III [1]. We develop a numerical algorithm to recognize and study the skyrmion filaments as the key constituents of the BPIII,. We show the difference between the half-skyrmions which form in thin planar cell geometry and the quarter-skyrmion filaments in thicker samples or in 3D bulk geometry. The distribution of the radial twist of the director relative to the distance to the skyrmion centre shows a continuous span of values, generally corresponding to half-skyrmions in thin planar cell geometry and quarter-skyrmion filaments in thicker cells and in bulk.
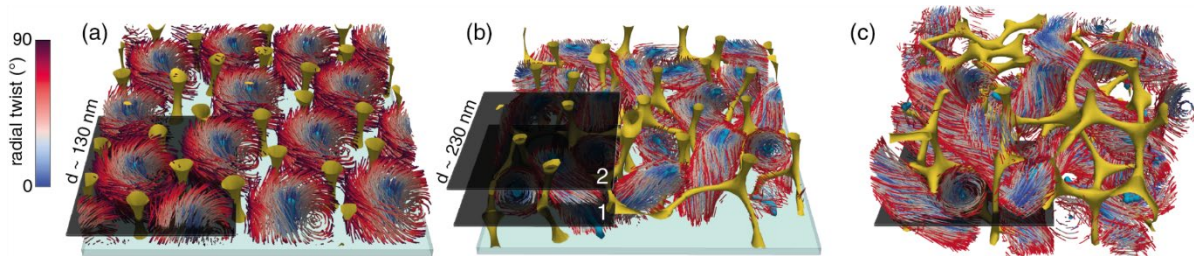
Figure 1: The BPIII skyrmion structures in thin planar cell (a), thick cell (b) and in bulk (c). The centre of the skyrmions are shown in light blue. BPIII skyrmions are visualized using vector field lines representing the director field, colored according to the local radial twist with respect to the center of the skyrmion. The color bar for the radial twist is shown on the left. The disclination lines are shown in yellow. The bottom plate, where planar anchoring condition applies, is shown with light blue, whereas the top plate is omitted for clarity.

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Numerical modeling of optical modes in topological soft matter

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Vector and vortex laser beams are desired in many applications and are usually created by manipulating the laser output or by inserting optical components in the laser cavity. Distinctly, inserting liquid crystals into the laser cavity allows for extensive control over the emitted light due to their high susceptibility to external fields and birefringent nature. In this work we demonstrate diverse optical modes for lasing as enabled and stablised by topological birefringent soft matter structures using numerical modelling. We show diverse structuring of light — with different 3D intensity and polarization profiles —, as realised by topological soft matter structures in radial nematic droplet, in 2D nematic cavities of different geometry and with different-charge topological defects, in arbitrary varying birefringence fields with topological defects and in pixelated birefringent profiles. We use custom written FDFD code to calculate emergent electromagnetic eigenmodes. Control over lasing is of a particular interest aiming towards the creation of general intensity, polarization and topologically shaped laser beams.

Analog of the Frank-Read Source in Nematic Liquid Crystals

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Under external stress, a pinned dislocation segment in a crystalline solid can deform and continuously generate dislocation loops, known as a Frank-Read source. We investigate an analogous mechanism of defect multiplication for disclination lines in nematic liquid crystals. We model a liquid crystal cell containing a disclination half loop pinned to one substrate via patterned surface anchoring, which is illustrated in Figure 1.
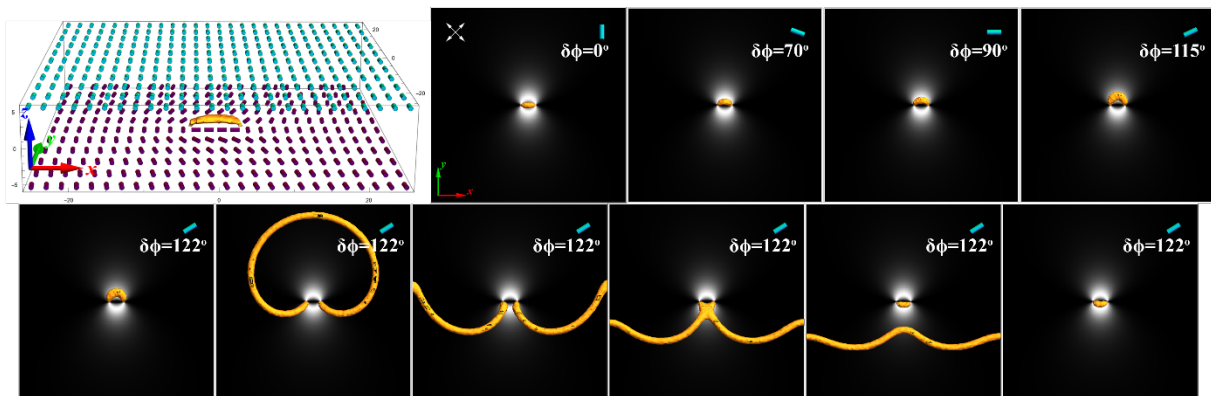

Figure 1: Illustration of the Frank-Read source model in nematic liquid crystals and our simulation results. The yellow lines in these graphs indicate the position of the disclination. The gray scale background is used to indicate the pattern on the bottom substrate.

External stress is imposed by gradually rotating the uniform planar anchoring orientation on the opposite substrate. As stress increases, the half loop stretches until a threshold stress is reached and a disclination loop is emitted, leaving the original pinned half loop intact such that the process can repeat. To understand this finding, we develop a simple theory based on the free energy of the system, and explain the behavior of this nematic Frank-Read source by the balance of the Peach-Koehler force and the tension of the disclination line. [1] In our latest finding, chirality in the liquid crystal also induces a bending effect on the pinned disclination which is similar to the effect from the rotated top substrate, and we demonstrate theoretically a chiral Peach-Koehler force emerging from a chiral nematic liquid crystal in addition to the regular Peach-Koehler force. We compare our findings to related experiments [2] and discuss implications for disclination nucleation mechanisms in both passive and active nematic liquid crystals.

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A numerical approach to liquid crystal texture analysis

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Extracting useful information from a texture image is a highly desirable and frequently used approach in many different fields and on different scales (e.g., cartography, biology and engineering). Valuable data can be obtained with suitable numerical analysis of the texture images, which is a discerning way of deriving information on subtle features of the studied material. For the past few decades, a number of texture analysis numerical methods have been proposed. The most well-known approach, due to Haralik, is based on the light intensity of individual pixels which involves a grey level co-occurrence matrix. Recently, this method has been generalized to encompass colour images, and a proposed further extension of this approach is discussed in this presentation.

The main aim of the presented approach is to obtain information about the sequences of mesophases present in thermotropic liquid crystals, and to focus on situations in which transitions between the mesophases are hardly identifiable by other methods. Issues related to the different arrangement of the individual pixels in the textures are investigated, exploiting the directional dependence of some of the Haralik characteristics. Examples of coloured textures obtained with a polarizing-microscope, in which the sequence of ferroelectric smectic and blue phases occur, will be shown, together with the results of the numerical analysis of these images. It will also be shown that the method may be useful in determining the influence of an external electric field e.g., through the change in observed wavelength in the liquid crystal blue phases.

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Chirality and polarity of relaxation modes in the ferroelectric SmC^* phase

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In this contribution we re-consider characteristics of the relaxation modes in the chiral ferroelectric SmC^* phase. We refer to these characteristics as a nature and a character of a relaxation mode: if the fluctuations in a perturbed system are related to the predominant changes of the tilt, the nature of the mode is tilt, and if the fluctuations are related to the predominant changes of the polarization, the mode is polar in nature. Furthermore, if the fluctuations are related to the changes of the magnitude, the character of the mode is amplitude, and if the fluctuations are related to the changes of the phase, the mode is phase in character. In addition, in a chiral, tilted, polar system, fluctuations appear in two possible chiral configurations - out of which, one is energetically more favourable [1]. Therefore, relaxation modes also have chiral properties, and the chiral interactions result in gaps between the amplitude modes.

Polar modes in chiral tilted smectics were predicted several decennia ago [2]. It was found that in the SmC^* phase the amplitude fluctuations in the behave as a Soft linearly dependent on the temperature, whereas orientational fluctuations in the Goldstone mode are temperature independent and recover the continuous symmetry broken at the phase transition temperature. However, later detailed analysis of relaxation modes that include the polar modes has shown a non-linear temperature dependence of both, tilt and polar modes [3]. Since both types of modes change their nature from the tilt to the polar and vice versa, we show that usually used relation [4] between the frequency and the amplitude of a relaxation mode in dielectric measurements $\varepsilon''\omega = const.$ is correct only if mutual orientations of tilt and polarization fluctuations are considered strictly orthogonal. As fluctuations of polarization are not strictly perpendicular to the tilt fluctuations, the product $\varepsilon''\omega$ depends on the temperature.

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Active coarsening dynamics

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Active nematics are systems base on self-propelled building blocks that exhibit orientational ordering, often characterized by the emergence of topological defects which can be spontaneously created or annihilated [1]. In this work we focus on the coarsening dynamics of active nematic system in three-dimensional active turbulence regime, where the defect density varies mainly due to the expansion and shrinking of defect loops. Our simulations are based on the Beris-Edwards approach to nematodynamics which are numerically integrated using the hybrid lattice Boltzmann method. We assume that active coarsening dynamics could be produced by changes in activity or by phase transition from isotropic to active nematic phase.

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Electrooptical effect of laser photobleaching on viscoelastic properties in chiral liquid crystals

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The viscoelastic properties are one of the most fundamental properties of the chiral liquid crystals. In general, their determination is not a straightforward task, however. The main problem is multitude of the physical parameters need to determine the value of the elasticity and viscosity constants [1]. It is also necessary to take into account the character of a respective phase. This problem is particularly important in the case of chiral phases such as ferroelectric and antiferroelectric, or in the blue phases.

There are experimental methods for measuring viscosity and elasticity constants in chiral phases, which exploit various phenomena to detect deformation, e.g. a light transmission, polarization current, light modulation, dielectric constant and helix deformation or helix unwinding. Commonly, in measurements an external electric field is applied to induce deformation and the homogeneity of the electric field inside the cell is of essential importance.

In this presentation we focus on the analysis of the effect of laser photobleaching on the electro-optical properties of the tested ferroelectric liquid crystal, and on the behavior of the electric field homogeneity before and after the procedure. The results obtained by confocal microscopy, enabling the observations of the electric field strength as a function of the cell depth, have been presented. The influence of the stabilization procedure of the isolated region performed by controlled laser photobleaching on the electro-optical properties has been compared with measurements taken before the photobleaching procedure.

The observation has been conducted with a polarizing microscope and simultaneously with use of the method of numerical analysis of two-dimensional coloured textures. The obtained results suggest that laser photobleaching can produce the enhanced electric field homogeneity and an anchoring boundary, which have a positive effect on the electro-optical properties.

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Determining the Kerr constant in blue phases

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Blue phases (BPs) are a chiral type of liquid crystalline state which are complex assemblies of double-twisted cylinders separated by defect lines. Three types of BPs are known: amorphous BPIII and two phases organized in cubic fashion, simple cubic BPII, and body centred cubic BPI. They are formed between the isotropic and cholesteric phases in narrow temperature range, although recently they have been stabilized over much broader range what has opened up possible applications of BPs in next-generation displays and in photonics. Potential applications of BPs liquid crystals are based on their optical isotropy and the electro-optical Kerr effect, which provides submilliseconds switching time.

In the Kerr effect the induced birefringence is proportional to square of the electric field intensity and the Kerr constant plays a key role in determining the electro-optic properties of BPs. In particular, this is directly related to operation voltage. Consequently, the knowledge of the Kerr constant of BPs is of great relevance, but its determination is still not a simple task.

In this presentation, a method for determination of the electro-optical Kerr constant is presented. We consider an approach for determining the Kerr constant which is based on measurement of electric-field-induced birefringence with linear detection of the modulated ac component of the transmittance intensity. The experimental results show that the scheme allows for a fairly accurate estimation of the Kerr constant. Moreover, the results determined from corresponding Gerber's formula is compared. Also, the numerical analysis of the textures has been applied as a complementary method to measure the induced birefringence in the studied materials.

Optical Second Harmonic Generation in Ferromagnetic Liquid Crystals

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Optical second harmonic generation (SHG) is an important method for resolving structural polarity of different liquid crystalline (LC) phases [1]. In this contribution we examine magnetic field-induced polarity in ferromagnetic LCs. A comparative experimental investigation of the dependence of SHG signal on an applied electric field and on an applied magnetic field between the standard nematic LC and a ferromagnetic nematic LC was performed [2]. A ferromagnetic LC was obtained as a mixture of a standard LC with ferromagnetic nanoplatelets [3]. The signal observed in the standard LC is attributed to a combination of electric field-induced and flexoelectric deformation-induced SHG, while the signal observed in the ferromagnetic LC is attributed solely to the flexoelectric deformation-induced SHG (Fig.1). The obtained results show that both contributions generate about the same effective polarity.
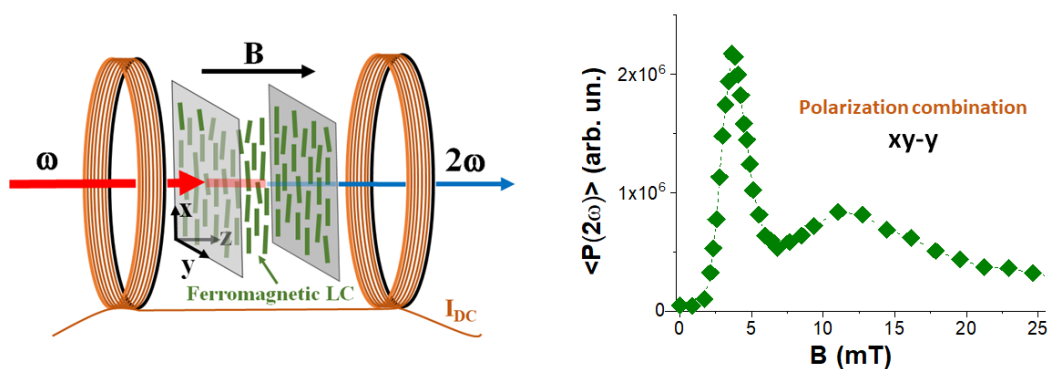

Fig. 1. Schematic drawing of the experimental setup (left) and SHG signal <P(2ω)> as a function of the applied magnetic field B (right).

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Hydrodynamic coupling in ferromagnetic cholesteric liquid crystals

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Liquid crystals (LC) are well-known for their strong responses to the external electric fields and strong external magnetic fields, E and B. These responses are typically invariant to the change of sign of the applied fields. Different is the case of ferromagnetic liquid crystals (FLCs). Here the magnetic nanoplatelets are suspended in the LC-media and the system is described by two coupled order parameters, the director and magnetization, i.e. average orientation of suspended magnetic nanoplatelets [1]. The coupling between the order parameters is such that parallel orientation is energetically most favourable. In this case the material is sensitive to the sign of the externally applied magnetic field (the situation for E remains the same here). Since the magnetization changes sign under time reversal, various static and dynamic phenomena, uncharacteristic for the usual LCs, have been observed [2].

Cholesteric LC (CLC) are chiral versions of the nematic LC (NLC). While the energetically favourable structure of NLCs is aligned configuration in the orientational order, the CLCs form helical structures, due to the chirality of the doped constituents. Analogously with the ferromagnetic NLCs, it is possible to make ferromagnetic cholesteric liquid crystals (FCLC), which also exhibit a strong response linear in the magnetic field [3]. In the case of FCLCs, the dynamic of the response is no longer invariant to the sign of external electric field E when the external magnetic field is also applied. This is due to the additional inversion symmetry breaking obtained by introducing chirality into the system. Terms linear in E and B appear in hydrodynamic equations and so the dynamic response of the material may now depend on the sign of E [4].

Experiments using polarising optical microscopy were performed in order to detect the described effect in the presence of external E and B applied perpendicularly one to another. The material was placed in layer confinement with perpendicular anchoring on the layer boundaries. Differences with respect to the polarity of E were observed in the starting reorientation dynamics from the magneto-optic response.

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Nitrophenyl end-capped bent-core liquid crystals

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Bent-core liquid crystalline materials have been intensively studied due to their unique properties and a variety of mesophases. Type of the formed phases (nematic, smectic, polar smectic SmCP, and columnar phases) could be modified by the variations of the mesogenic core, lateral substitutions, the character of linkages and terminal chains. Recently we studied the role of the terminal arylalkyl chains on the mesomorphic properties and found that the presence of the aromatic unit at the end of the molecular tail did not disturbed the ability to self-assemble and the nematic and B-type phases were observed. [1]

Herein, we present a structurally new type of aryl-terminated bent-core liquid crystals (Figure 1) with a polar nitrophenyl moiety connected to an aliphatic terminal chain of variable length (n=4-12). The studied compounds showed a complex polymorphism of liquid crystalline mesophases: nematic and multiple smectic phases were detected. For the phase temperatures, an even-odd effect was observed with respect to the length of the linker (n number). The textures in smectic phases exhibited a regular array of stripes (Figure 1), resembling those observed in twist-bend nematic and smectic phases. [2] Observed stripes represent a regular pattern and acted as diffraction gratings in polarised light.

We analysed the studied compounds by various experimental methods. We performed x-ray measurements and established the layer spacing value temperature dependences within the smectic mesophases.
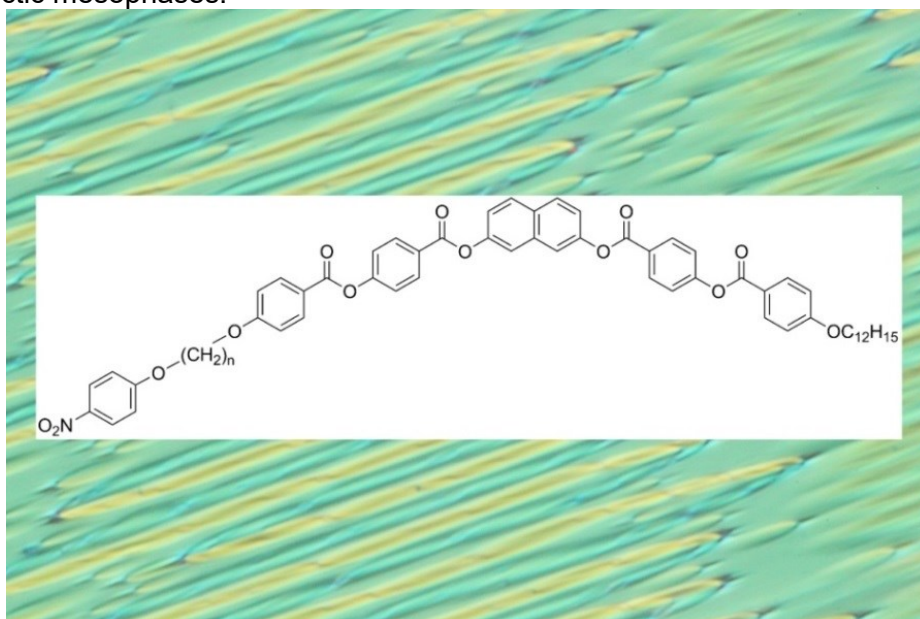

Figure 1: Chemical formula of the studied materials. In background, there is the stripe texture observed in the SmA phase for one homologue.

References:
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Dielectric properties of synclinic and anticlinic smectic in enantiomeric and racemic version

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Synclinic ferroelectric and anticlinic antiferroelectric smectics exhibit reach dielectric responses. For enantiomer, one strong mode (Goldstone mode) is observed in SmC* while two collective weak modes P_L and P_H are detected in SmC$_A$*. One suggests that collective modes in SmC$_A$* are weak because they are almost canceled due to anticlinic packing in neighboring layers. Additionally, molecular S-mode (rotation around a short molecular axis) exists in both: enantiomeric and racemic anticlinic phase. When the DC field is applied to SmC* the Goldstone mode is suppressed because the helix is unwound. Simultaneously both P_L and P_H modes are slightly strengthened by the DC field. When racemate is investigated the Goldstone mode in SmC is completely suppressed due to the absence of the helix. Surprisingly only P_H mode is completely suppressed in SmC$_A$ while P_L mode still is electrically active. In racemic mixture in SmC new weak mode (named X mode) is observed. This mode seems to be the continuation of P_L mode. When the DC field is applied to racemate one can see that P_L (in SmC$_A$) and X mode (in SmC) are strengthened by the DC field. We investigated the compound (enantiomer S, and racemate(R,S)) synthesized (MU) at our university (figure 1):
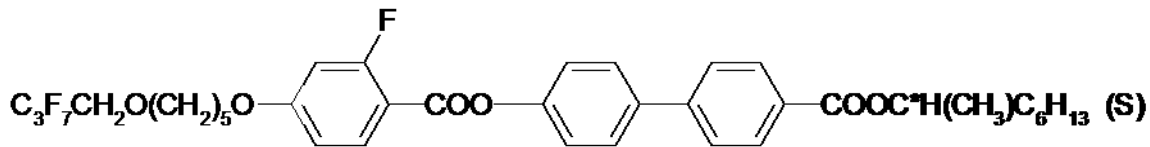

Figure 1. The molecular structure of the investigated compound.

In figure 2 the permittivity $\varepsilon'_\perp$, measured in HG, 5μm cells with gold electrodes, is presented for enantiomer (a) and racemate (b) under DC field.
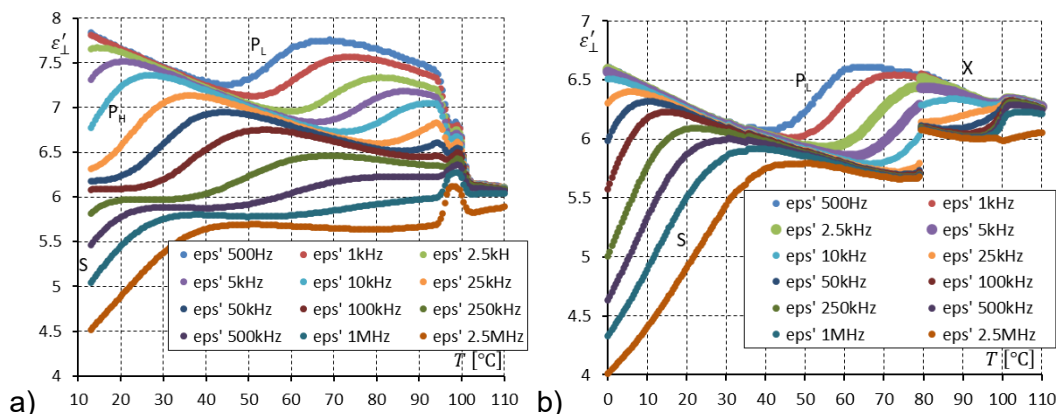

Figure 2. Permittivity versus temperature for 12 measuring frequencies in enantiomer (a) and racemate (b)

For all modes (measured with and without DC field) their relaxation parameters were calculated using our model. The obtained results are discussed.

Tuning nematic ordering of barium-hexaferrite nanoplatelets in 1-butanol

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Spontaneous ferromagnetic nematic ordering of barium hexaferrite nanoplatelets (NPLs) in isotropic solvents happens above a certain threshold concentration [1]. The result is a special example of a dipolar fluid – a liquid magnet. The interactions that are the driving force for the ferromagnetic nematic phase formation are long-range magnetic and screened anisotropic electrostatic interactions. The dipolar magnetic interactions arise from the ferrimagnetic NPLs with the magnetic easy-axis perpendicular to the plate's plane, while the electrostatic interactions are present due to the surfactant dodecylbenzenesulphonic acid [2]. The surfactant enables the colloidal stability of the suspensions at threshold concentrations. Here, we present how the NPLs' diameter, the strength of magnetic and electrostatic interactions, and the screening of electrostatic interactions affect the phase behaviour of the suspensions and the threshold concentration. The phase behaviour of the suspensions was studied by polarized optical microscopy (Figure 1). We observed that the threshold concentration decreased with the increasing average mean diameter or saturation magnetization of the NPLs or with the increasing ionic strength of the suspension [3].

Figure 1: Magnetic domains in a ferromagnetic nematic suspension of BHF NPLs.

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Reinvestigation of superlattice structures in an extraordinary phase sequence of a ferroelectric liquid crystal using adiabatic scanning calorimetry

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The ferroelectric liquid crystal compound, namely nOHFBBB1M7 (n = 10) exhibits an extraordinary phase sequence in which superlattice structures have been analyzed by the Landau model and the partially molecular model in the past [1-3]. Herein, we reinvestigate this extraordinary phase sequence using the Peltier-element-based Adiabatic Scanning Calorimetry (pASC), impedance spectroscopy, and polarized optical microscopy. The pASC revealed no signature of the SmC_{F12}^* phase in between the SmC^* and SmC_α^* phases; however, a remarkable superheating effect is observed. We have extensively discussed the pros and cons of all the models within the scope of this study.
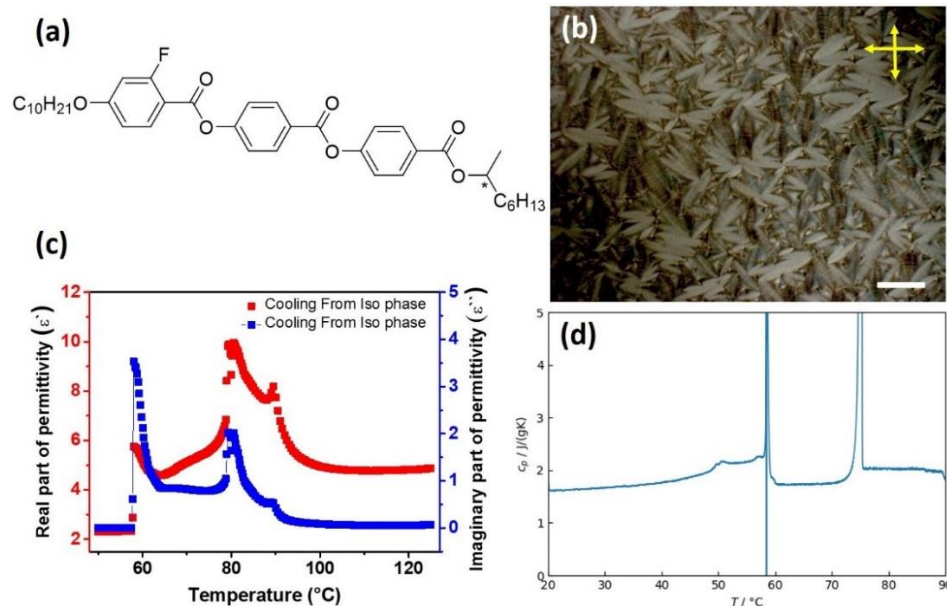
Figure 1: (a) Molecular structure of 10 OHF, (b) POM image at 55 °C, (c) real and imaginary parts of dielectric permittivity as a function of temperature, and (d) pASC scan using P=100 μW.

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Ferroelectric nematics as associating polymers

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We have carried out atomistic simulation studies of the recently discovered ferroelectric nematic (N_F) phase [1-3] in an effort to identify the key features of molecular interactions and correlations responsible for polar order in N_F materials. Comparative simulations of polar and nonpolar states of the N_F mesogen RM734 reveal distinct polarity-dependent intermolecular correlations (Figure 1B-E) and characteristic polar and antipolar pair association motifs (Figure 1F-K), and show that the polar state of RM734 is more energetically stable than the nonpolar state (by ~ 0.16 kcal/mol per molecule). The most prominent features in the pair distributions can be traced to attractive, polarity-dependent electrostatic interactions between specific functional groups (e.g., between nitro and terminal methoxy groups in Figure 1F). Such electrostatic 'bonds' lead to the formation of polar associated polymer chains and networks in both the nonpolar (N) and polar (N_F) states. This may significantly reduce the entropy cost of global polar orientational order, enabling a small energetic preference for the polar state to stabilize the N_F phase at low temperatures. Further support for this 'associating polymer' paradigm comes from simulation studies of a number of RM734 analogs.
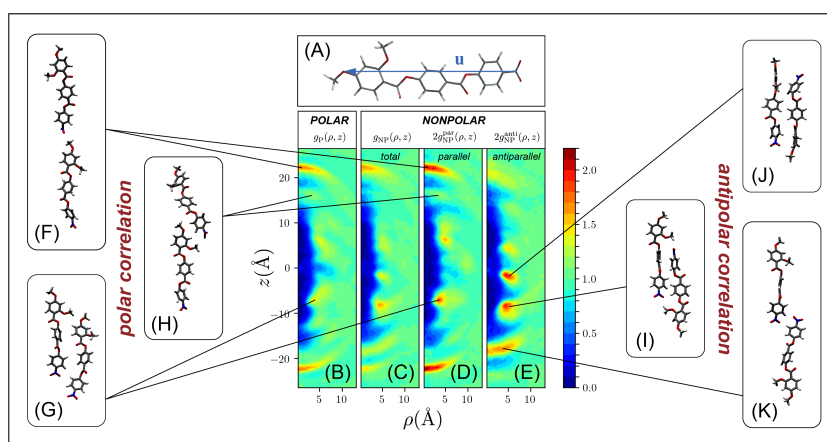

Figure 1: Results from atomistic simulations of RM734 at $T = 130°$C. (A) Molecular structure of RM734 and definition of the polar molecular director $\mathbf{u}$. (B-E) Azimuthally-averaged pair distribution functions $g(\rho, z)$ in a molecule-fixed reference frame defined by the polar director $\mathbf{u}$ of the molecule centered at the origin ($+z$ direction), where ρ and z are the radial and longitudinal pair separations, respectively. For the nonpolar system the total $g(\rho, z)$ (C) is resolved into contributions from parallel (D) and antiparallel (E) pairs. Characteristic polar and antipolar pair correlation motifs associated with prominent features in $g(\rho, z)$ are shown in (F-H) and (I-K), respectively, including head-to-tail 'chaining' (F) and polar transverse correlations involving the lateral methoxy group (G and H).

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Ferromagnetic Nematic Phases of Charged Magnetic Nanoplatelets

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In recent decades, advances in synthesis techniques have opened up a new subfield in the study of magnetic soft matter: the study of anisotropic and anisometric magnetic colloidal suspensions. The persistent interest in investigating and refining anisotropic colloidal systems comes from the knowledge that colloidal anisometry can be used as an effective control parameter to tune both self-assembly scenarios and thermodynamic, rheological and phase behavior of dipolar (magnetic) soft matter[1]. For instance, it is now possible to synthesize discotic mesogens with a dipole moment perpendicular to the long axis of the particle. This combination of anisotropy and anisometry results in a suspension which can form a macroscopic ferromagnetic nematic phase at room temperature[2].

While the phase behavior of hard platelets is already well-known, the influence of the added dipole moments, platelet size polydispersity and electrostatic repulsion on the isotropic to nematic phase transition are not yet fully understood. Bringing together experimental investigations of the suspensions, theoretical predictions and simulations, we aim to characterise the phase behavior of such systems in detail. This contribution will focus on the computational work, recreating the system through Molecular Dynamics simulations in different approximations (raspberry and Gay-Berne), then studying the influence of parameters such as the dipole moment or aspect ratio on the phase transition, as well as analysing the structural properties of the system in different phases.

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Separation of active-dipolar cubes at an obstacle in Poiseuille flow

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The term "active matter" describes a class of out-of-equilibrium systems, whose ability to transform environmental energy to kinetic energy is sought after in multiple fields of science. A challenge that still remains is the creation of nanometer sized active particles, whose motion can be effectively directed by externally applied stimuli. Adding a magnetic component and therefore being able to direct the motion of active nanoparticles with an applied magnetic field proofed promising and effective in previous experimental and theoretical investigations[1]. A common scenario that is envisioned for the use of active nano-particles is their controlled transport in micro- and nano-channels. The present study focuses on active-dipolar cubes that showed their capability of being directed by an externally applied magnetic field in a previous study[2]. We employ Molecular Dynamics simulations coupled to an explicit Lattice Boltzmann fluid to simulate a channel with a thermalized Poiseuille flow and a cylindrical obstacle inside (Figure 1a). We test the particles and their probability to pass the object on a certain side that is determined by the direction of the applied magnetic field. We find that the efficiency of that process depends on the ratio between the active force and the flow velocity, as well as the particle internal configuration of active force and dipole orientation. The results allow us to predict the circumstances under which an active particle is magnetically controllable in flow, making it more accessible to technical and medical applications.
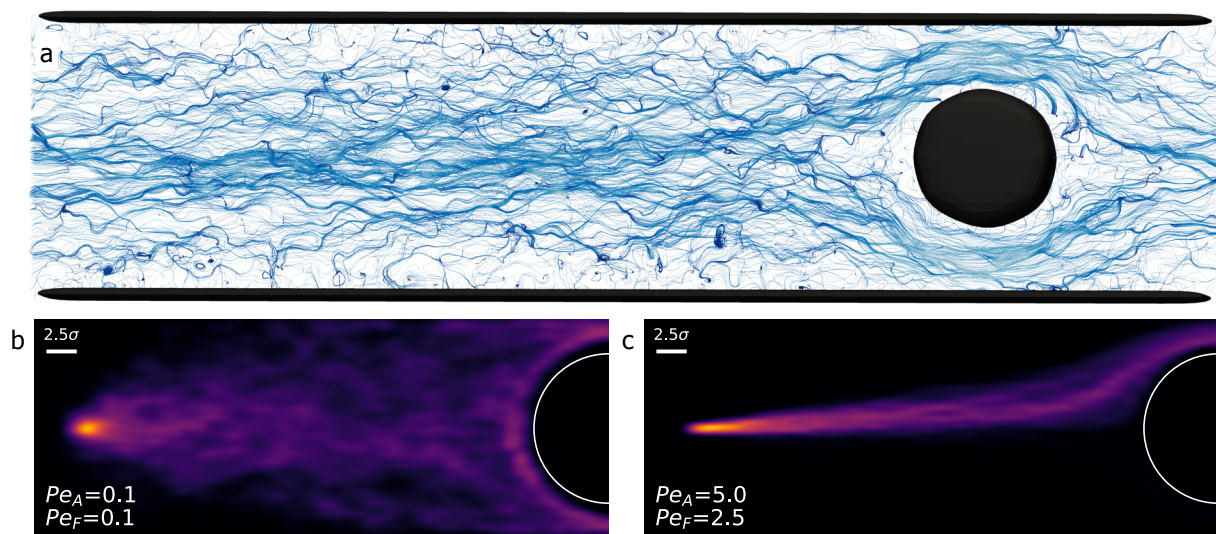

Figure 1: a: Visualization of a thermalized Poiseuille flow in a channel with a cylindrical obstacle inside. Note that the active-dipolar particle is not visualized in this figure. b&c: Heatmap of positions of active-dipolar cubes in a channel visualized in (a). Pe_A denotes the Péclet number of the active particle, Pe_F the Péclet number of the fluid.

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Characterization of nano-polymers synthesized through directional assembly of DNA nano-chambers

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Polymer stimuli-responsive materials are one of the central research topics in modern soft-matter physics. Responsiveness to magnetic fields is particularly appealing for technological and bio-medical applications in which active control of the materials behaviour is required, due to the highly dynamic control on the intensity and the spatial resolution that is possible to achieve with these stimuli. Construction of smart materials with sophisticated magnetic response by incorporating magnetic nanoparticles within permanently cross-linked structures (i.e. magnetic filaments), opens up the possibility for synthesis of more complex, highly magneto-responsive systems.[1,2] Recent advances, advocating an assembly mechanism where the structure building instructions are embedded into nanoparticles via DNA origami frames, finally open the door towards synthesis of such materials with tuneable magnetic response mechanical properties. It has been shown that a pre-defined set of different DNA-framed nanoparticles, along with DNA polyhedral frames, enable designing diverse planar constructs, 1D, 2D and 3D frameworks. [3,4] Although it is well understood that sophisticated hierarchical structures could be assembled by programing the dimensionality, specificity and strength of connections between with DNA polyhedral building blocks, other intrinsic properties of connections are not explored. Some tunable properties are highly relevant to morphologies of large-scale organizations, and mechanical properties of the lager superstructures they form.

Using a combination of experiments and molecular dynamics computer simulations, we present how tunable properties, namely the length and arrangement of DNA linkers of DNA nano-chamber polyhedral frames reflects itself on morphologies of large-scale organizations. More specifically we demonstrate that by tuning the aforementioned properties, one can achieve assembly into polymer-like, linear nanofiber structures. We use computer simulations to predict equilibrium properties of the arising structures for a broad range of lengths and rigidities, elucidating the impact of the monomer shape.

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