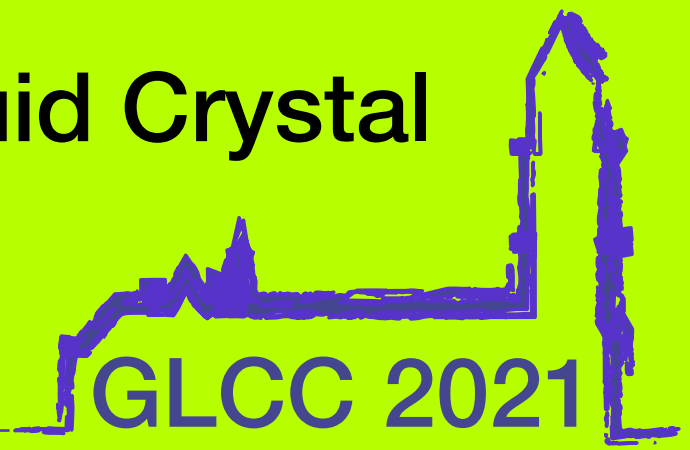


47th German Liquid Crystal Conference



Magdeburg, March, 17 2021 -
March, 19 2021

A circular inset showing a microscopic image of a liquid crystal phase. The image displays a complex, textured pattern with various colors including red, orange, yellow, green, and blue. The texture appears to be a combination of fine, granular structures and larger, more distinct shapes, possibly representing different phases or defects in the liquid crystal. The overall appearance is highly detailed and colorful.

Advances in
Soft Matter
Physics

47TH GERMAN LIQUID CRYSTAL CONFERENCE, MAGDEBURG 2021

SCIENTIFIC PROGRAM

Dear Participants,

On behalf of the German Liquid Crystal Society and the Local Organizing Committee, we welcome all participants to the 47th German Liquid Crystal Conference. This year, we are confronted again with the pandemic situation. The chances to organize a conference where scientists and students can meet personally are out of scope. A virtual conference relates to a real conference only like a concert on CD, listened to at home, to a concert in a great music hall. No matter how well it is prepared, it can only be a substitute. Nevertheless, we are doing our best to make this virtual meeting a success. This conference primarily offers young scientists the opportunity to present their results, to discuss, and to learn from experienced international researchers. The German Topical Meeting on Liquid Crystals (Arbeitstagung Flüssige Kristalle) has a long tradition. It has long become an international-scale workshop promoting an exchange of views among scientists working with Soft Matter and, in particular, liquid crystals.

In fact, the first meeting of this conference series, the 1. Freiburger Arbeitstagung Flüssige Kristalle, took place almost exactly 50 years ago, on April 23, 1971. Since then, it took place annually for five decades, with very few interruptions in years when large international conferences were organized in Germany, and last year when the outbreak of the COVID-19 pandemic forced us to cancel the meeting.

The organizers ask you for your understanding, for flexibility, forbearance, and tolerance in case some things will not run perfectly well.

There are a couple of special issues that you should observe during the meeting. They are detailed on the next page. We wish you an exciting and stimulating meeting.

The organizers of GLCC2021,

Alexey Eremin,

Andreas Menzel,

Ralf Stannarius

Technical and organizational details

First and foremost, there will be a message board with information for all attendees. You find it on the conference web site

<http://www.liquidcr.ovgu.de/glcc2021/messageboard.html> .

This website contains all the relevant information. In case of any unforeseen interruptions, events, or technical problems, we will inform you on this website about actions to take. In case you have any questions regarding the program or related issues, send an email to

GLCC20@OVGU.DE .

The local organizing committee will respond as soon as possible.

The conference will be held entirely in the form of Zoom Meetings. Make sure that you have installed the most recent Zoom application on your computer or that you can access Zoom Meetings with an appropriate browser on your computer. If you log in to the sessions, you must do so with your first and last name, or, at least, with your last name and initials. Make sure that you have a camera ready. You do not need to log in with the video switched on, but on request, you must be able to show your video. This is to avoid uninvited clients in the sessions. Participants who do not log in using their name tags, or cannot show their video on request, will be removed from the sessions. With the Meeting Passcode, you have open access without the necessity to wait for an approval by the host at entry. Should we encounter problems with this open entry scheme, we might have to change it during the conference. Please, strictly mute your microphone, unless you are explicitly asked to speak by the session chair.

The Meeting IDs and Passcodes will be sent only to the conference attendees. Do not distribute this information to third parties. On each day, we will start one single Zoom Meeting, which will run for the whole day. For each day, we have separate Passcodes, which you will receive by email.

In order to avoid technical complications, we have decided that each session is chaired by a local chairperson. We hope that you understand. The chairperson will strictly obey the conference schedule. When you are presenting, please be prepared to start right after the chairperson calls you. Please, check your internet connection and audio/video systems in advance. Delays due to technical problems will not be compensated for.

Presenters of a Short talk plus Poster have the option to discuss their posters in special breakout sessions. At the respective poster discussion, you enter the breakout room assigned to your poster and you have time to answer questions of all participants who enter your breakout room. There will be 3 poster discussion sessions with 40 minutes each and 12 posters in each session. Contributions labeled S##/P## are those with Short talks and Posters, contributions labeled S## only are Short talks without posters. We will also provide virtual (Zoom) rooms for communications.

All posters emailed to the conference organizers will be removed from the website and deleted no later than Monday, March 22. The organizers will take measures to obviate unauthorized access to the conference documents. Nevertheless, we cannot guarantee that your uploaded posters are absolutely safe from access by a professional or deliberate intruder, or from redistribution by other conference attendees. Please keep this in mind when preparing your files and act in a way that appears reasonable to you.

Conference Schedule

WEDNESDAY, March 17, 2021

08:45	Opening	(Organizers)	
	Session We1	(Eremin)	
09:00-09:30	I1	Fumito Araoka	Functional properties in doped polar nematics
09:30-09:50	O1	Muhammad Ali	Spontaneous formation of polarization diffraction gratings in the twist-bend nematic phase
09:50-10:10	O2	Lawrence Honaker	Nematic liquid crystal interfacial tensions: an anisotropic issue
10:10-10:30	O3	Anjali Sharma	Liquid crystal elastomer shells with exotic actuation modes programmed by topological defects
	Session We2	(Stannarius)	
11:00-11:30	I2	Rebecca Walker	Structure-property relationships, chirality and the twist-bend nematic phase
11:30-12:30	S01/P01-S12/P12	SHORT TALKS 1	
12:30-14:00	Lunch Break		
	Session We3	(Harth)	
14:00-14:30	I3	Jordi Ignés-Mullol	Active nematic liquid crystals under confinement: flow control, synchronization, frustration, and active boundary layers
14:30-14:50	O4	Berteloot Brecht	From planar patterned photoalignment to vertical alignment in 3D-ring shaped liquid crystal structures
14:50-15:10	O5	Sergey Shvetsov	Light beam action on dye-doped liquid crystal film with free surface
15:10-15:30	O6	Atefeh Habibpourmoghadam	Generation of optical vortices in context of a nematic liquid crystal assisted by anomalous electrical properties of ITO
	Session We4	(Menzel)	
16:00-16:20	O7	Florian Malotke	Photonic sensing based on supramolecular liquid crystals: halogen/hydrogen bond competition in liquid crystal sensors
16:20-17:20	S13/P13-S24/P24	SHORT TALKS 2	
17:30-18:10	P01-P12	POSTER DISCUSSIONS	
18:15-18:55	P13-P24	POSTER DISCUSSIONS	
	Vorländer I	(Kitzerow)	
19:30-20:30	V1	Andreas Menzel	Emergent dynamic liquid-crystalline order in active crowds

THURSDAY, March 18, 2021

	Session Th1	(Nadasi)	
09:00-09:30	I4	Vladimira Novotna	Lactate derivatives exhibiting re-entrancy phenomenon and nanotube formation in the crystalline phase
09:30-09:50	O8	Meik Blanke	Properties of natural polyphenolic compounds as building blocks for supramolecular liquid crystals
09:50-10:10	O9	Martin Lambov	Stable-radical supermesogens for potential magnetic applications
10:10-10:30	O10	Subrata Nath	Tuning the solid-state emission of liquid crystalline nitrocyano stilbene by halogen bonding
	Session Th2	(Stannarius)	
11:00-11:30	I5	Corinna Maaß	Nematic droplet swimmers
11:30-12:30	S25/P25-S36/P36	SHORT TALKS 3	
12:30-14:00	Lunch Break		
	Session Th3	(Menzel)	
14:00-14:30	I6	Miha Ravnik	Ionically charged topological defects in nematic fluids
14:30-15:30	S37-S48	SHORT TALKS 4	
	Session Th4	(Nadasi)	
16:00-16:20	O11	Evangelia Zavvou	Dielectric response of symmetric ether-linked cyanobiphenyl liquid crystal dimers
16:20-16:40	O12	Małgorzata Jasiurkowska-Delaporte	Molecular dynamics and crystallization behavior of liquid crystals in bulk and nanometric confinement
16:40-17:00	O13	Pravinraj Selvaraj	Superior electro-optic response in organic N-benzyl-2-methyl-4-nitroaniline doped in nematic liquid crystal device
17:05-17:45	P25-P36	POSTER DISCUSSION	
	Saupe-Award	(Kitzerow)	
18:00-19:00	Saupe-Laureate	Antal Jakli	Liquid crystal spherical caps in magnetic and electric fields
	Vorländer I	(Kitzerow)	
19:30-20:30	V2	Verena Görtz	Modulated and confined nematic liquid crystals

FRIDAY, March 19, 2021

	Session Fr1	(Eremin)	
09:00-09:20	O14	Sonja Dieterich	Synergistic structures in lyotropic lamellar gels
09:20-09:40	O15	Artur Geivandov	Deformed lying helix transition in cholesteric LC layers at spatially periodic boundary conditions
09:40-10:00	O16	Wojciech Tomczyk	Generalized Landau-de Gennes theory of the twist-bend nematic phase: on the role of flexopolarization
	Session Fr2	(Menzel)	
10:30-11:00	I7	Alenka Mertelj	Polar nematic phases
11:00-11:20	O17	Mohamed Alaasar	Photosensitive fluorinated hydrogen-bonded polycatenars
11:20-11:40	O18	Paulina Rybak	Characterisation of strongly fluorescent mesogens with quinoxaline based cores
11:40-12:00	O 19	Piotr Lesiak	Modelling of self-organizing photonic structures based on nematic liquid crystals
12:00-13:00	Lunch Break		
	Session Fr3	(Harth)	
13:00-13:20	O20	Christina Abele	Particle size dependent phenomena in lyotropic graphene oxide liquid crystals
13:20-13:40	O21	Pawel Pieranski	Fréedericksz transition on air
13:40-14:10	I8	Helena Godinho	Oscillating cellulose-based structural colors
14:10	Closing	(Organizers)	

Abbreviations:

- I Invited talk (30 min incl. discussion)
- O Regular talk (20 min incl. discussion)
- S/P Short talk (5 min incl. discussion) / Poster presentation (40 min)
- V Vorländer Award Lecture (60 min)

Short Talks and Posters Schedule

Name	Affiliation	Title	S/P
Short talks: We 11:30		Poster session: We 17:30	
Simdyankin, Ivan	FSRC Crystallography and Photonics RAS Moscow	Spatially localized electrooptical modes in vertically aligned nematic LCs	S01/P01
Klopp, Christoph	OvGU	Coalescence of liquid droplets in a quasi 2D liquid film	S02/P02
Kitzerow, Heinz	Paderborn University	Electro-optical addressing of meta-surface based optical tweezers	S03/P03
Schmidtke, Jürgen	Paderborn University	Cholesteric ring resonators	S04/P04
Loiko, Valery	Institute of physics of NAS Belarus Minsk	Polymer dispersed liquid crystal films doped with carbon nanotubes: modeling of the electrooptical response	S05/P05
Gerbig, Lisa	University of Wuerzburg	The “click-procedure” extended to porphyrin star mesogens	S06/P06
Černá, Tereza	University of Chemistry and Technology Prague	Design and synthesis of liquid-crystalline dimers exhibiting B4 phase	S07/P07
Fryń, Paryk	Jagiellonian University Kraków	Influence of single-walled carbon nanotubes and liquid crystal 5CB admixtures on physical properties of L,D-PLA	S08/P08
Noll, Katja	Universität Würzburg,	Controlling the liquid-crystalline phase by ionic guests	S09/P09
Haege, Christian	University of Stuttgart	Understanding the phase behavior of ionic liquid crystals: the role of the charge position - a simulation study	S10/P10
Scheuring, Nikolai	University of Wuerzburg	Approaching the holy grail of liquid crystal science - biaxial nematic phases from roof-shaped mesogens	S11/P11
Herzog, Anselm	University of Würzburg	Synthesis and characterisation of a PBI substituted oligothiophen-star mesogene	S12/P12
Short talks: We 16:20		Poster session: We 18:15	
Weinberger, Pascal	Universtiy of Wuerzburg	Systematic study of ionic liquid-crystalline tricyanoborates forming smectic mesophases	S13/P13
Baumann, Maximilian	University of Wuerzburg	Umbrella-shaped LC star subphthalocyanines - E-field orientable polar mesophases	S14/P14
Ivanov, Viktor	MLU-Halle	Orientationally ordered structures in a single flexible-semiflexible multi-block copolymer chain: flat histogram Monte Carlo simulation	S15/P15

Prasad, Aparna	University of Wuerzburg	Siloxane decorated star-shaped phthalocyanines as low clearing functional liquid crystals.	S16/P16
Šmahel, Michal	University of Chemistry and Technology, Prague	Photosensitive liquid crystals derived from 4-halogenoresorcinols	S17/P17
Perkowski, Paweł	Military University of Technology, Warsaw	Electric properties of ferro- and antiferroelectric phases in racemic mixture	S18/P18
Grunwald, Marco	Universität Stuttgart,	Synthesis of star-shaped alkoxy- and chloro-triphenylbenzenes: Suzuki coupling in the presence of halogenated precursors	S19/P19
Klopp, Christoph	OvGU	Coarsening dynamics of 2D emulsions in quasi 2D fluids	S20/P20
Drzewicz, Anna	Polish Academy of Sciences Kraków	Study of a novel chiral glass-forming liquid crystal	S21/P21
Deptuch, Aleksandra	Polish Academy of Sciences Kraków	Relationship of cold crystallization kinetics and molecular dynamics in 3F5HPhH compound	S22/P22
Filimonova, Evgeniia	MLU-Halle	Molecular origin of the heterogeneity in the nematic and smectic liquid crystals: elastic constants, gradients of order parameters and visualization of small objects	S23/P23
Piwowarczyk, Marcin	Polish Academy of Sciences Kraków	Mesomorphism and photochemistry of (E)-4-((4-decyloxyphenyl)diazenyl)phenyl alkanoates	S24/P24
Short talks: Th 11:30		Poster session: Th 17:05	
Ramou, Efthymia	NOVA University of Lisbon,	Using cyanobiphenyl-based liquid crystal droplets to detect volatile gases	S25/P25
Nordendorf, Gaby	Paderborn University	Surface modification with benzophenone derivatives for liquid crystal test devices	S26/P26
Kasyanova Irina	Russian Academy of Sciences	Electrically tunable diffraction and anomalous refraction by metasurfaces made of nematic liquid crystal	S27/P27
Dardas, Dorota	Polish Academy of Sciences Poznan	Rheological properties of ferroelectric liquid crystalline materials	S28/P28
Belyaev, Victor	Moscow Region State University	Luminescent, dielectric and contact properties of liquid crystal composites with multilayer quantum dots	S29/P29

Bruckner, Johanna	University of Stuttgart	Tailored lyotropic liquid crystal templates: chances and limitations of added co-surfactants and swelling agents	S30/P30
Mamuk, Atilla Eren	Mugla Sitki Kocman University, TURKEY	Investigation of electrospun liquid crystal/polymer nano-fibers: effect of liquid crystal type	S31/P31
Stebryte, Migle	ELIS department, Ghent University	Large angle forward diffraction by chiral liquid crystal gratings with inclined helical axis	S32/P32
Busch, Mark	Hamburg University of Technology	Structure of the liquid crystal C8BTBT with high-charge-carrier mobility confined in hydrophilic and hydrophobic anodic aluminium oxide nanochannels	S33
Raszewski, Zbigniew	Military University of Technology, 00-908 Warsaw	Nematic liquid crystals for light transducers with high-transmission of light and very low reflection at visible, near, short and medium infrared regions	S34
Tykarska, Marzena	Military University of Technology Warsaw	Inversion of helical twist sense in three component system showing SmC*A phase	S35
Lalik, Sebastian	Jagiellonian University Kraków	Influence of the ferroelectric BaTiO ₃ nanoparticles on some properties of the antiferroelectric binary mixture	S36
Short talks: Th 14:30		no posters	
Zhang, Bingru	Paderborn University	Aggregation properties of a chromonic liquid crystal	S37
Becker, David	Universität Paderborn	Influence of the annealing conditions and the host materials on a columnar liquid crystal based OLED	S38
Benkowska-Biernacka, Dominika	Wroclaw University of Science and Technology	Lyotropic liquid crystals stained with Nile Red	S39
Duda, Łukasz	PORT Polish Center for Technology Development	Intermolecular proton transfer between liquid crystalline chiral 4-phenylpyridine derivative and organic acids	S40
Ebert, Max	Universität Stuttgart	Self-assembly of aminocyclopropenium salts: en route to deltic ionic liquid crystals	S41
Zieja, Paulina	Military University of Technology Warsaw	Induction of smectic A phase in mixtures of nematic compounds showing positive and negative dielectric anisotropy	S42

Juszyńska-Gałązka, Ewa	Polish Academy of Sciences Kraków	Odd-even effect in homologous series of 4-cyano-3-fluorophenyl 4'-nbenzoates (nCFPB)	S43
Galazka, Mirosław	Polish Academy of Sciences Kraków	Electric conductivity and electric polarisation of electrodes as markers of phase transitions	S44
Chrzanowska, Agnieszka	Kraków University of Technology	Can Onsager theory describe smectic liquid crystals ordering?	S45
Singh, Dharmendra Pratap	Université du Littoral Côte d'Opale (ULCO)	Charge transport properties in hybrid discotic matrix amalgamated with 0D nanostructured materials	S46
Patel, Mehzabin	University College London	Temperature-induced liquid crystal microdroplets and templated microparticles in a partially miscible liquid mixture	X47
Starzonek, Szymon	Polish Academy of Sciences	Complex dynamics and phase behaviour of liquid crystals under pressure	X48

Invited Talks

Second Harmonics Microscopic Imaging to Visualize Flexoelectric Polarization

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Even-order nonlinear optical (NLO) effects are useful to probe symmetry-broken states because they are prohibited in centrosymmetric systems due to the parity transformation rule which dictates electronic transitions. One of such NLO effects, optical second harmonic generation (SHG), is useful in material researches for its feasibility to optically access the spontaneous/induced polarization possessed by the light-transmitting media. More specifically in liquid crystal (LC) researches, SHG is often used to know the molecular orientation, symmetry and switching dynamics in ferroelectric/antiferroelectric LC phases or the microscopic molecular ordering at surfaces/interfaces [1]. Meanwhile, owing to the recent development of the sensitive imaging techniques, now we are able to spatially resolute the optical signals even at the single photon level. Therefore, now the SHG microscopy is becoming an affordable technique to visualize the local symmetry breaking or the distribution of the internal electric field of the dielectric/semiconducting materials, i.e. the local distribution of induced/spontaneous polarizations [2].

In this presentation, first, a technical overview of the SHG microscopy for LCs will be given with some examples of visualization of spontaneous polarization in ferroelectric LCs. Followingly, we will demonstrate visualization of the flexoelectric polarization in nematic LCs in which SHG has been conventionally thought to be forbidden because of their centrosymmetric nature. The flexoelectric effect is a coupling of elastic deformation and electric dipoles [3], which deteriorates the image quality by the so-called image flickering effect, in particular, being significant in the fringe-field switching (FFS) mode [4]. In the present work, the flexoelectric polarization is induced by applying an external electric field to various nematic LCs with positive or negative dielectric anisotropy, including a cholesteric LC. We also make a comparison of SHG images among various cell geometries not only of FFS but also of in-plane switching (IPS) and twisted nematic (TN) modes. Furthermore, we have confirmed the flexoelectric polarization even in the blue phases (BPs) using a wide-temperature BP material without polymer-stabilization. Thus, we believe that our method is greatly advantageous to evaluate the performance of industrial LCDs, influenced by the design of devices and LC materials.

[1] I.-C. Khoo and S.-T. Wu, *Optics and Nonlinear Optics of Liquid Crystals*, World Scientific, Singapore (1993).

[2] T. Manaka et al., *Nat. Photonics*, 1, 581 (2007).

[3] R. B. Meyer, *Phys. Rev. Lett.*, 22, 918 (1969).

[4] M. S. Kim et al., *Sci. Rep.*, 6, 35254 (2016).

Structure-Property Relationships, Chirality and the Twist-Bend Nematic Phase

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²Department of Chemistry, University of Warsaw, ul. Zwirki i Wigury 101, 02-089 Warsaw, Poland

The experimental identification of a new nematic phase in 2011 is undeniably one of the most significant developments of the past decade in liquid crystal science.[1], [2] The twist-bend nematic phase, N_{TB} , is at present restricted to liquid crystal materials which are typically – but as we will see, not exclusively – achiral and, fundamentally, have a sufficiently bent molecular structure. In the N_{TB} phase, the molecules arrange in a heliconical superstructure of nanoscale periodicity, while retaining a random distribution of their centres of mass. Unlike the cholesteric phase, N^* , for which the director twists around an axis perpendicular to the long axes of the molecules, the director in the N_{TB} phase is tilted at a constant angle $\theta < 90^\circ$ and precesses on a cone forming an oblique helix of pitch about two orders of magnitude shorter than that found in the N^* phase, and equal to just 2-3 molecular lengths.[3]–[5] The N_{TB} phase can be considered as a generalised case of the N^* phase and has been described as the ‘structural link’ between the N and N^* phases. Undoubtedly the most fascinating feature of this phase is that this chiral superstructure is formed despite its constituent molecules being chemically achiral, and indeed the N_{TB} phase represents the first example of such spontaneous chiral symmetry breaking in a fluid system with no spatial ordering. As this induction of chirality is spontaneous, there exists an equal probability of formation of either handedness of helix and hence the N_{TB} phase constitutes doubly degenerate locally chiral domains of opposite handedness, giving a globally achiral phase.

Here we present a range of new liquid crystal dimers which exhibit the N_{TB} phase and discuss structure-property relationships.[6]–[8] We also consider the effect of molecular chirality on the formation of the N_{TB} phase.[9] Finally, we will discuss the recent observation of twist-bend smectic phases and how these relate to molecular structure.[10], [11]

[1] I. Dozov, *Europhys. Lett.*, vol. 56, no. 2, pp. 247–253, 2001.

[2] M. Cestari *et al.* *Phys. Rev. E - Stat. Nonlinear, Soft Matter Phys.*, vol. 84, no. 3, pp. 1–20, 2011.

[3] D. Chen *et al.* *Proc. Natl. Acad. Sci. U. S. A.*, vol. 110, no. 40, pp. 15931–15936, 2013.

[4] V. Borshch *et al.*, *Nat. Commun.*, vol. 4, pp. 1–8, 2013.

[5] C. Zhu *et al.*, *Phys. Rev. Lett.*, vol. 116, no. 14, 2016.

[6] R. Walker *et al.*, *Soft Matter*, vol. 15, no. 15, pp. 3188–3197, 2019.

[7] R. Walker *et al.*, *Chem. Commun.*, vol. 54, no. 27, pp. 3383–3386, 2018.

[8] D. A. Paterson *et al.* *Liq. Cryst.*, vol. 45, no. 13–15, pp. 2341–2351, 2018.

[9] R. Walker *et al.*, *Chem. - A Eur. J.*, vol. 25, no. 58, pp. 13329–13335, 2019.

[10] J. P. Abberley *et al.*, *Nat. Commun.*, vol. 9, no. 1, pp. 1–7, 2018.

[11] M. Salamończyk *et al.*, *Nat. Commun.*, vol. 10, no. 1, 2019.

Active nematic liquid crystals under confinement: flow control, synchronization, frustration, and active boundary layers

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²PMMH and Laboratoire Gulliver, UMR CNRS 7083, ESPCI Paris, PSL Research University, 75005 Paris, France.

Unlike traditional nematic liquid crystals, which adopt ordered equilibrium configurations compatible with the topological constraints imposed by the boundaries, active nematics are intrinsically disordered because of their self-sustained internal flows [1]. Here, we show that confining a kinesin/tubulin active nematic to circular or annular microfluidic channels enables controlled directional flows and autonomous transport [2]. In single annular channels, the typically chaotic streams can be transformed into well-defined circulating flows, whose direction or handedness can be controlled by introducing asymmetric corrugations on the channel walls. The dynamics is altered when multiple annular channels are interconnected, leading to scenarios of synchronization, anti-correlation, and frustration of the active flows, and to the stabilization of high topological singularities. Finally, we find that, under slip boundary conditions, the channel wall induces the accumulation of negatively charged topological defects in its vicinity, resulting in the formation of a topological boundary layer that polarizes the wall [3]. While the dynamics of wall and bulk defects are decoupled, we find that the active boundary layer influences the overall dynamics of the system, to the point of fully controlling the behavior of the active nematic in situations of strong confinement

[1] Doostmohammadi, A., Ignés-Mullol, J., Yeomans, J. M., Sagués, F. *Active nematics*. Nature communications **9**, 3246 (2018).

[2] Hardoüin, J., Laurent, J., Lopez-Leon, T., Ignés-Mullol, J., Sagués, F. *Active microfluidic transport in two-dimensional handlebodies*. Soft Matter **16**, 9230 (2020).

[3] Hardoüin, J., Laurent, J., Lopez-Leon, T., Ignés-Mullol, J., Sagués, F. *Active boundary layers*. arXiv:2012.02740.

Lactate Derivatives exhibiting Re-entrancy Phenomenon and Nanotube Formation in the Crystalline Phase

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Prague, Czech Republic

² Chemistry Department, Warsaw University, Al. Zwirki i Wigury, Warsaw, Poland

We present liquid crystalline compounds, which reveal the thermotropic mesomorphic properties with a rich variety of mesophases [1-2]. Studied compounds consist of a molecular core laterally substituted by a chlorine atom, and we modified both terminal chains (Figure 1a). We concentrated on the effect of the terminal alkyl chain in the chiral part. For selected homologues both enantiomers were synthesised and racemic mixtures prepared. We studied the mesomorphic behaviour and for one homologue a reentrancy of the SmA phase below the tilted SmC phase was detected, for both chiral enantiomers as well as for the racemic mixture. For chiral compounds with the SmC* phase, ferroelectric properties were studied by dielectric spectroscopy and switching properties were described. Reentrancy of the SmA phase was experimentally proved by several experimental techniques including x-ray measurements. For racemic mixtures we measured the birefringence and analysed the behaviour at the phase transitions.

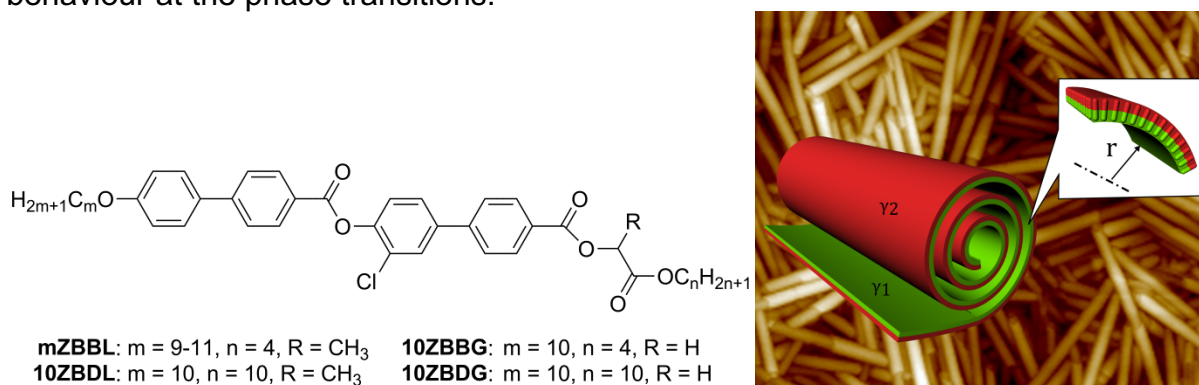


Figure 1. a) Chemical formula of studied compounds and b) for homologue 10ZBBL the nanotubes in the crystalline phase, detected by AFM, and a scheme of nanotube formation.

We found that for selected homologues we can prepare the nanotubes by slow evaporation from a solution [3], at the room temperature in the crystalline phase. For lactate derivatives both enantiomers as well as the racemic mixtures formed the nanotubes. We observed that the nanotube formation is not dependent on the solvent, concentration or deposition surface type. Obtained supramolecular assemblies were studied using AFM, TEM and SEM techniques, other experimental techniques (IR, UV-Vis spectroscopy and x-ray diffraction) were applied. The difference in the surface tension at the opposite crystallite surfaces is suggested as a possible mechanism for the nanotube nucleation (Figure 1b) on evaporation from solution.

References:

- [1] V. Novotna, et al., Journal of Materials Chemistry, **21**, 14807–14813 (2011).
- [2] N. Podoliak, et al., Physical Review E, **84**, 061704 (2011).
- [3] V. Novotna, et al., Nanoscale Adv. **1**, 2835-2839. (2019).

Nematic droplet swimmers

Babak Vajdi Hokmabad, Carsten Krüger, Kyle Baldwin, Christian Bahr, Corinna Maass

Max Planck Institute for Dynamics and Self-Organisation, Göttingen

Self propelling microswimmers are of great interest for soft and active matter physics, both with respect to their biomimetic properties, e.g. their use as synthetic cell models, as well as for their potential in microengineering smart materials. Here, swimming droplets are a highly promising class of active agents, which, despite their simple and tunable design and easy fabrication, show a wealth of features based on fundamental principles of non-equilibrium physics, nonlinear dynamics and spontaneously broken symmetries [1].

Using a nematogen as the droplet material, we can harness nematic topology and its coupling to liquid crystal elasticity to add more features to the swimmers.

Nematoelasticity enables us to generate helically swimming droplets [2], non-coalescing liquid shells that can be used as microcarriers [3], and droplets steered by external magnetic fields.

- [1] C.C. Maass et al., *Annu. Rev. Condens. Matter Phys.* **7**, 171–193 (2016).
- [2] C. Krüger et al., *Phys. Rev. Lett.* **117**, 048003 (2016).
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Ionically Charged Topological Defects in Nematic Fluids

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Controlling the electric charge in liquid electrolytes is of prime importance in a range of applications such as supercapacitors, or the self-assembly of particles in colloidal or biological settings. However, realizing localised charge profiles in the bulk of such electrolytes generally requires the presence of surfaces which poses a fundamental constraint on the material design. Here, we show using numerical modelling that nematic topological defects in nematic electrolytes can perform as regions for local charge separation, forming charged defect cores and, in some geometries, even electric multilayers, analogous to electric double layers found in isotropic electrolytes. Specifically, we show that flexoelectricity and ion solvability perform as the main mechanisms for the effective charging of the nematic. Different bulk and surface geometries will be discussed, including flat interfaces and colloids. More generally, the relevance of this work is for possible applications where topological defects act as diffuse ionic capacitors or as ionic charge carriers.

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Polar nematic phases

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In the last decade, polar nematic has been observed in three different systems. Ferromagnetic ordering appears in suspensions of magnetic nanoplatelets in thermotropic non-chiral or chiral nematic liquid crystals (NLC) [1,2] and isotropic solvents [3,4], while ferroelectric order emerges in thermotropic nematic materials made of wedge-shaped molecules with large electric dipole moments [5,6].

I will discuss recent advances in research of these phases. In particular, I will focus on phase transitions to polar nematic phases. I will discuss the suspensions of magnetic nanoplatelets in isotropic solvents, and show how electrostatic magnetic interactions between the nanoplatelets affect the transition from isotropic to ferromagnetic nematic phase. In the second system, which is a thermotropic nematic material, the experiments show that the phase transition from the ordinary nematic to the ferroelectric splay nematic phase is a ferroelectric-ferroelastic transition, in which flexoelectric coupling causes the simultaneous occurrence of diverging behavior of electric susceptibility and instability towards splay deformation.

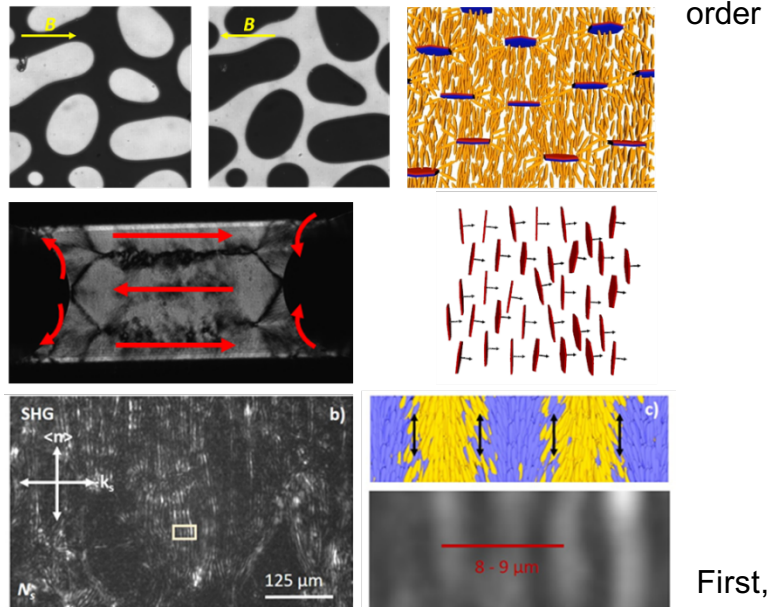


Figure 1: magnetic domains and schemes of suspension of magnetic platelets in an NLC (top) and in an isotropic solvent (middle). SHG image and scheme of modulated splay nematic structure which appears at the phase transition (bottom).

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Oscillating cellulose-based structural colors

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Cellulose and cellulose derivatives are very well known to form lyotropic cholesteric phases [1]. These solutions can display different colours depending on the solvent concentration, pressure and temperature [2]. The wavelength reflected by the sample depends not only on the cholesteric pitch but also on the refraction index of the mesophase and the observation angle, accordingly to de Vries equation [2, 3]. Increasing the concentration of the solvent normally increases the value of the pitch [2]. However, many of cellulose-based fundamental properties are still not explored and poorly understood. Among the most remarkable characteristics of cellulose is its chirality, which translates into cellulosic right and left-handed structures [4, 5]. In this work we focus on cholesteric cellulosic systems, which form lyotropic phases in “reactive solvents”, with vivid colors for a given range of concentrations, at room temperature. The spatio-temporal evolution of the pitch of encapsulated thin layers, was followed in time. The results were analysed taking into account diffusion-reaction gradient models [5].

Acknowledgements

This work is funded by FEDER funds through the COMPETE 2020 Program, National Funds through FCT - Portuguese Foundation for Science and Technology and POR Lisboa2020, under the projects numbers POCI- 01-0145-FEDER-007688 (Reference UID/CTM/50025), UID/BIA/00329/2013, PTDC/CTM-BIO/6178/2014, M-ERA-NET2/0007/2016 (CellColor) and PTDC/CTM-REF/30529/2017 (NanoCell2SEC).

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Award Lectures

Vorländer Lecture V1

Emergent dynamic liquid-crystalline order in active crowds

Andreas Menzel

Investigations on orientational ordering touch the heart of the field of liquid crystals. For decades, an increasing number of symmetry classes has been revealed, analyzed, and in various cases led to overwhelmingly successful applications. Instead of pure “static” directions of liquid crystalline molecules, given for example by molecular axes, active agents feature additional “dynamic” directions as well, namely their velocities. To a big extent, the rapidly growing field of active matter is devoted to the study of collective effects resulting from orientational ordering of these dynamic directions. We review basic models developed to study the emergent dynamic ordering based on explicit alignment rules. Moreover, we concentrate on recent works on hydrodynamically mediated alignment interactions resulting for active microswimmers in suspension and on the onset of collective motion in regular structures on planar substrates. Considering the many facets of self-propelled synthetic or biological agents, the field of active matter has the potential to develop to similar significance as the field of liquid crystals itself.

Modulated and Confined Nematic Liquid Crystals

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The nematic phases formed by bend mesogens have provoked considerable interest because of their remarkable modulated characteristics.

In this talk, I will review our investigations of achiral bent-core nematic materials and will discuss our observations, such as domains of opposite handedness in conjunction with phase biaxiality, in context to the modulated twist-bend and splay-bend nematic phases.

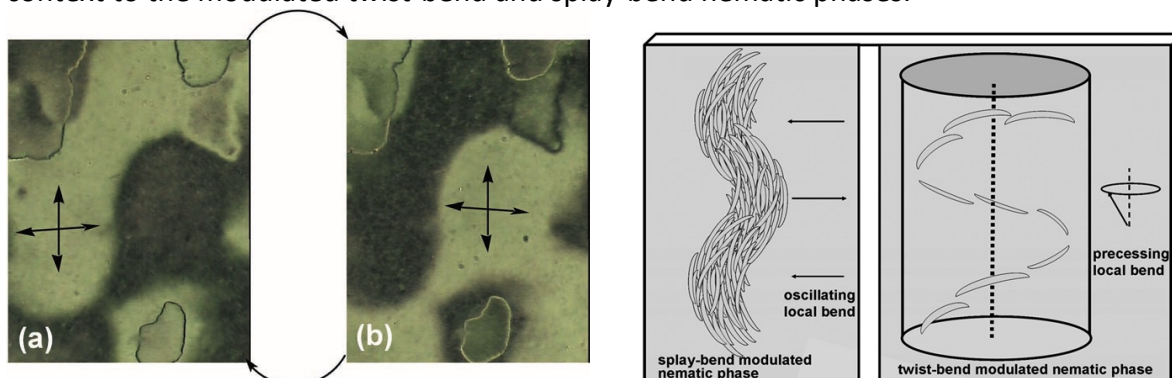


Figure 1. Domain segregation and modulated nematic phases of bent-core molecules.

A three-dimensionally curved shape is responsible for the characteristic confinement topologies and modes of self-organisation within colloidal nematic droplets and polymer particles.

In the second part of my talk, I will show how we use heterogeneous synthetic methods and careful monomer design to control topologies in nematic and chiral nematic polymer and elastomer particles, and how they translate into optical or mechanical responses that provide mechanisms for sensing and actuation.

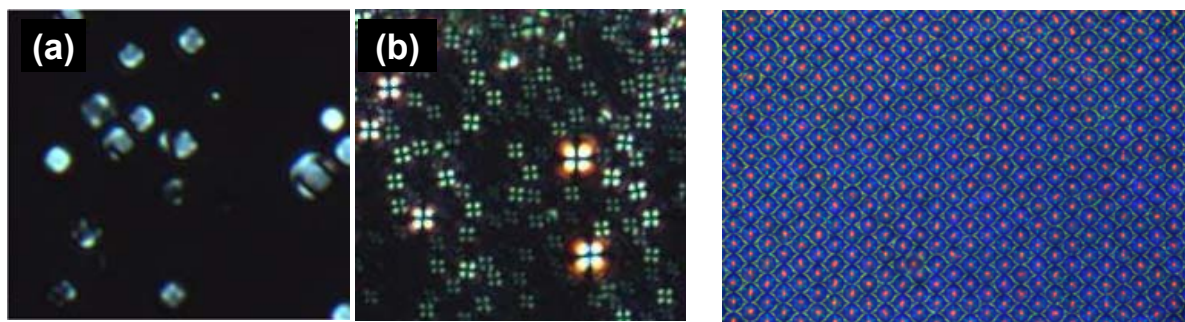


Figure 2. Photomicrographs of a) bipolar nematic, (b) radial nematic ($\sim 2\text{-}5\ \mu\text{m}$) and c) chiral nematic particles ($\sim 60\ \mu\text{m}$).

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Saupe-Award Lecture

Liquid Crystal Spherical Caps in Magnetic and Electric Fields

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Spherical cap shaped liquid crystal drops have a potential for their use in tuneable multifocal optical lenses. To achieve this, one needs to understand the liquid crystal director structure in various external fields.

We present detailed experimental and theoretical studies of the director structure of less than 1 mm diameter liquid crystal drops forming spherical cap shapes with homeotropic boundary conditions under DC magnetic^[1] and AC electric fields. We show that above a threshold field, a Néel wall-type metastable inversion wall forms in the middle of the drop and then moves outward (see Figure 1). In magnetic fields and in low frequency electric fields, the wall stays perpendicular to the field and moves along the field. Under high frequency electric fields, the wall rotates by 90° either to the left or right, while drifting to toward the periphery.

We present a theory that explains the texture variation in small fields and account for the formation of the inversion walls above a threshold. The theory explains the magnetic field and low frequency electric field dependences of the movement and gives the right magnitude of the speed.

The rotation of the defect wall at high frequency electric fields is a result of the antiparallel orientation of the effective moment vector and the electric field due the lower dielectric constant and higher electric conductivity of the defect wall than of the rest of the liquid crystal droplet.

Uniform electric field induced generation, rotation and linear movement of defect walls is a unique phenomenon in soft matters.

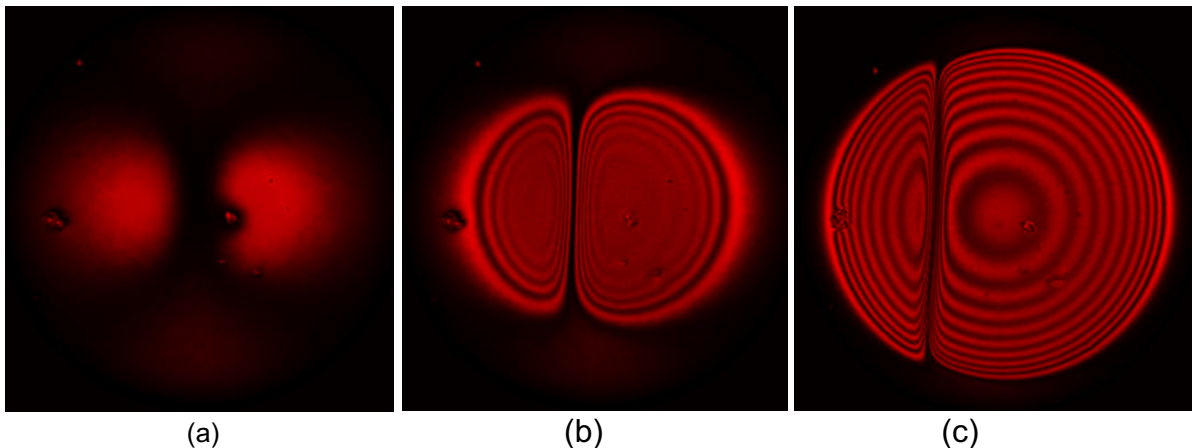


Figure 1: Typical textures of a 912 μ m diameter 8CB drop in various magnetic fields and times. (a) $H=0.5\text{kOe}$; (b) $H=1\text{kOe}$; (c) $H=10\text{kOe}$ 20 min after formation.

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Oral Presentations

Spontaneous formation of polarization diffraction gratings in the twist-bend nematic phase

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The properties of polarization diffraction gratings that are formed spontaneously in planar cells filled with a liquid crystal exhibiting a twist-bend nematic phase (N_{TB}) are studied both experimentally and theoretically. Due to the short-pitch heliconical modulation of the long molecular axes, the N_{TB} phase behaves as a pseudo-layered medium. Below the nematic (N) – N_{TB} phase transition temperature, the heliconical pitch and thus the thickness of the pseudo-layer reduces, which leads to a two-dimensional undulation of layers: in the direction perpendicular to the surfaces (vertical chevron) and along the surfaces (horizontal chevron). Under a microscope, a stripe texture is observed with the modulation period of twice the cell thickness [1]. Such a modulation acts as diffraction grating [2] (Fig. 1). We propose a continuum model to describe the formation of gratings as a result of competition between surface conditions and bulk strain due to shrinking of pseudo layers. We determine the threshold conditions for two-dimensional undulations of pseudo-layers. We measure the polarization states of the first two orders of the diffracted light and show that temperature dependence of the second order diffraction peaks is a sensitive tool to determine the spatial variation of the heliconical axis [3, 4]. We also propose a model to calculate the polarization state of the diffracted light. Theoretical predictions are in good qualitative agreement with the experimental observations. We use the transfer matrix method and beam propagation method to model the transmissivity of light by using the spatial variation of the optic axis determined from the continuum model [5].

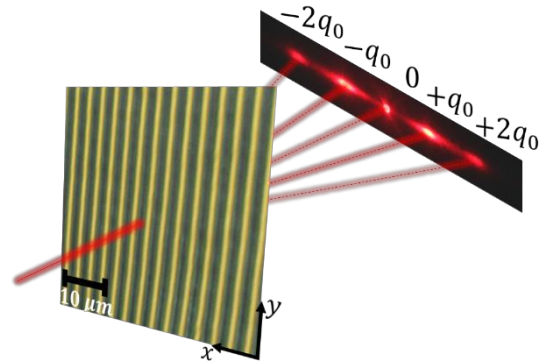


Figure 1: Stripe texture observed under microscope and corresponding orders of the diffracted light.

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Nematic Liquid Crystal Interfacial Tensions: An Anisotropic Issue

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Many properties of a liquid crystal phase, such as dielectric susceptibility and viscosities, show an alignment dependence. Interfacial tension is one such property that is thought to have an alignment dependence. However, liquid crystals such as 5CB are challenging to measure with classical interfacial tension methods [1] due to the sensitivity of these measurements to experimental data that are not well established or themselves alignment-dependent [2–4]. Additionally, quantifying the competing effects arising from surfactant behavior versus the realignment induced by a surfactant is not a trivial concern.

Here, using a recently-developed microfluidic interfacial tensiometry technique [5], we show the anisotropy between planarly and homeotropically aligned 5CB in the nematic phases. The case of homeotropic alignment is achieved by extrapolating a Szyszkowski equation [6] fit of sub-CMC interfacial tension data, while we can measure the planar interfacial tension with the presence of a polymer stabilizer that does not induce homeotropic anchoring. Where they exist, the data we obtain fit well to existing literature data. We additionally experimentally demonstrate that there is an anisotropy between interfacial tensions with planar and homeotropic alignment, which can, in turn, be used to determine the liquid crystal anchoring strength.

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Liquid crystal elastomer shells with exotic actuation modes programmed by topological defects

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Liquid crystal elastomers (LCEs) are highly attractive as soft actuators for, e.g., robotics, as they can dynamically change their shape in response to temperature changes, light or electric fields [1]. The mode of shape change can be powerfully controlled by introducing topological defects, as recently demonstrated by several authors [e.g. 2, 3]. Normally this is restricted to flat, relatively thin LCE films and it requires advanced patterning of sacrificial alignment layers, which are rejected after production. On the other hand, topological defects arise spontaneously in spherical shells of liquid crystal if the director field has a component in the plane of the shell [4]. This has been investigated extensively using low molar mass liquid crystals [e.g. 5-7] but only one study so far [8] reported *elastomeric* liquid crystal shells with topological defects. The LCE shell configuration is intriguing, both due to the spontaneous appearance of topological defects, and because—in contrast to LCEs made using standard methods—the ground state is already curved.

In [8] the shells were photocrosslinked *in-situ* during production, locking in a non-equilibrium director field with poor control of alignment and defect configuration. Two recent papers on LCE shells studied the case of equilibrium director fields [9-10], but in both cases the shells were radial, thus without topological defects.

In the present study, we prepare planar-aligned LCE shells from a monomeric precursor, separating in time the production from the polymerization. This allows us to stabilize an equilibrium defect configuration, typically with all defects collected near the thinnest point of the shell, prior to polymerization and crosslinking. Interestingly, the defect configuration as well as the shape change already *during* polymerization. Upon heating and cooling the resulting LCE shells, they show a reversible actuation behaviour defined by the topological defects [see Fig.1]. The motion is quite exotic, broken shells opening and closing in a jellyfish-like fashion, and all the shells rotating; stronger during actuation than during relaxation, thus breaking the symmetry.

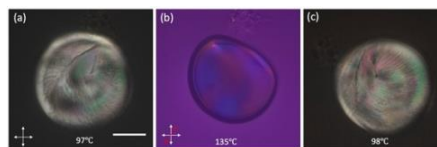


Fig.1: POM images of crosslinked shell at low temperature (a). Image (b) shows actuation on heating above the isotropic phase. On cooling below the isotropic phase, shell returns to the previous shape. Scale bar represents 50 μm .

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From planar patterned photoalignment to vertical alignment in 3D-ring shaped liquid crystal structures

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Liquid crystal (LC) can be aligned using linearly polarized blue or UV light that illuminates a photoalignment layer. The LC will align parallel to the glass substrate (planar) with the director oriented perpendicular to the orientation of the linear polarization. If both the top and bottom substrate of the LC cell define the same alignment orientation, the LC in the bulk of the cell will follow this alignment. If however both substrates define different alignment orientations, complex 3D structures can be formed in the bulk of the cell.

Using the projection of a spatial light modulator, we can define arbitrary LC alignment patterns. We used this setup to fabricate ring-shaped LC structures in which the nematic LC aligns vertically in the bulk of the cell, while the alignment is planar at the substrates.

The bulk director configuration of the fabricated cells has been investigated using Q-tensor simulations. These results were imported in optical transmission simulations and a good agreement was observed with polarization microscopy images of the fabricated cell. [1,2]

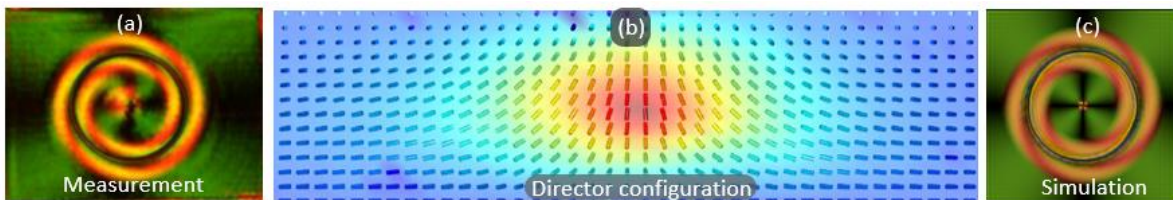


Figure 1: Microscope image of the fabricated sample (a). The director configuration is calculated using Q-tensor simulations (b). The director configuration is used to simulate the optical transmission of the structure (c).

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Light Beam Action on Dye-Doped Liquid Crystal Film with Free Surface

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Liquid crystals (LCs) represent unique optical materials. Because of their anisotropy and mobility, LCs are very sensitive to external fields. Light beam can cause a number of effects in a homogeneously oriented liquid crystal films. Light can cause, for example, the orientational torque due to optical anisotropy or dye dopant excitation [1].

Usually, the LC material is placed between two plane-parallel substrates which determine its alignment. Here we study the light interaction with LC film where one surface is in contact with the rigid substrate and another is in contact with air. This geometry is useful for investigating the thermocapillary and orientational effects (Fig 1a).

In this study, we used a mixture ZhKM-1277, which has a large thermal interval of nematic phase, doped with 0.4 wt % anthraquinone dye. The LC is placed onto the glass plate. The film thickness is evaluated to be 12 μm . Because of the orienting layer and LC-air interaction, it has a homeotropic alignment.

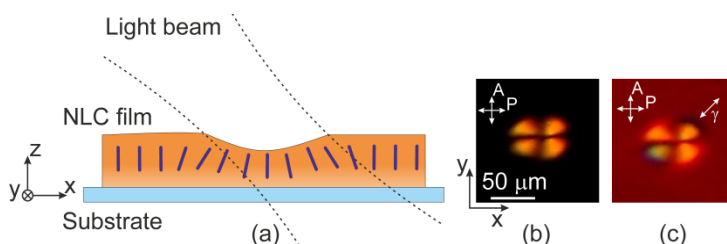


Fig. 1. The scheme of LC-light interaction (a); the images of irradiated area in crossed polarisers (b) and with additional λ -plate (c).

The focused light beam (the waist diameter is 64 μm) from a solid-state laser causes the local heating of LC film. At light beam power $P \sim 0.1$ mW, the aberrational pattern composed of centrally symmetric rings starts to form. The characteristic time of the pattern formation is 0.5 s. The analysis of the pattern formation [2] indicates the presence of negative nonlinearity (the decrease in the refractive index). The further increase in light beam power results in the cross pattern appearance in irradiated area (Figs. 1a and 1b). From this, we can assume that the surface and director field are deformed due to hydrodynamic flows at the thermocapillary effect.

The study was supported by the Russian Science Foundation, Grant No. 20-72-00178.

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Generation of Optical Vortices in Context of a Nematic Liquid Crystal Assisted by Anomalous Electrical Properties of ITO

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Indium-Tin-oxide ([In₂O₃:Sn], ITO) is often used as a transparent conducting electrode in liquid crystal (LC) cells. In non-plasmonic regime, ITO acts quite as a semiconductor supporting photo-generated charge carriers' redistribution and transport in its border interfaces with orientant or LC medium [1]. Rearrangement of photo-generated charge carriers at the light beam spot can significantly alter the static field distribution inside the LC cell, which in turn modulates the LC director field [1]. This is exploited in nematic LCs with positive dielectric anisotropy in the creation of wavefront singularities characterizing optical vortices (OVs) in incoming both linearly and circularly polarized plane waves by means of formation of umbilical defects (in short umbilics) [2]. Creation of helical waves from an incoming circularly polarized plane wave in the template of a radial umbilic (with topological charge of +1) is schematically shown in Figure 1a.

Creating stable and tuneable defect structures in the LCs for the purpose of generating controllable OVs has been a challenge over past decades. Recently, high efficiency (> 90%) LC light valves employing nematic LCs with negative dielectric anisotropy have been achieved by Kravets, et al [3].

In this work, instead of conventional LC light valves, LC cells made from a photosensitive slab, i.e, iron doped lithium niobate (Fe:LN) as the photovoltaic source generating electric field in the LC with positive dielectric anisotropy covered with an ITO coated glass plate were suggested (Figure 1b). It was shown that such hybrid cells filled with a nematic LC with positive dielectric anisotropy can act as an efficient context for the generation of OVs.

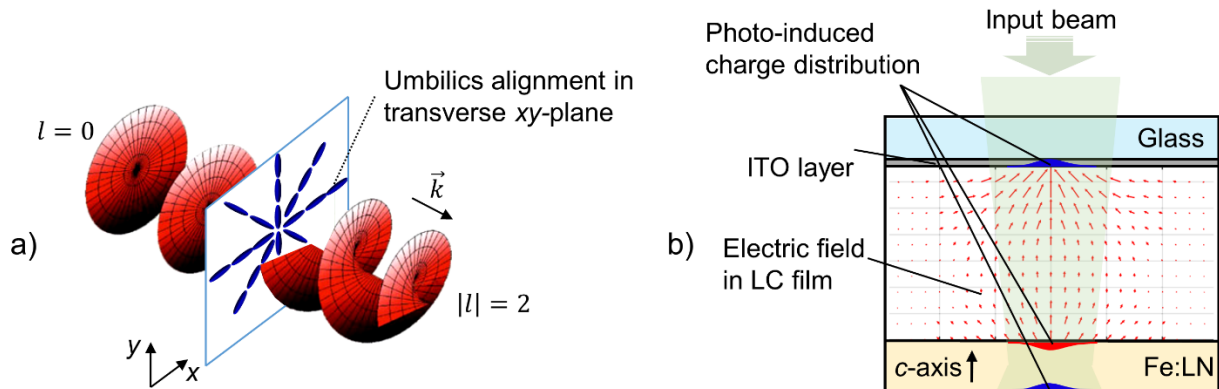


Figure. a) Nematic LC as a template for the generation of OVs through umbilics formation. l gives the helicity charge corresponding with orbital angular momentum of $|l|\hbar$ per photon. b) Electric field distribution in the LC film modified by phot-generated charge carriers' redistribution in the ITO thin layer.

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Photonic sensing based on supramolecular liquid crystals: Halogen/Hydrogen bond competition in liquid crystal sensors

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Colouration is omnipresent in nature and plays a fundamental role in perception of signals.^[1] The partial-periodic nanostructure and the associated Bragg-reflection of supramolecular cholesteric liquid crystals (CLCs) provides an excellent corner pillar for the preparation of the aforementioned materials.^[2] These one-dimensional photonic crystals present an intrinsic sensitivity towards external stimuli, owing to the reversible nature of the non-covalent interactions.^[3] Exploiting the hydrogen bond for supramolecular purposes and self-assembly has been subject to a multitude of studies for decades, whereas the usage of halogen-bonding has only gained attention more recently.^[4] Seminal studies targeting hydrogen and halogen-bond interaction strengths lead to the conclusion that both binding types can be addressed in a single material. Based on a supramolecular modular concept,^{[5][6]} hydrogen-bonded liquid crystalline complexes have been developed, exhibiting liquid crystallinity at room temperature which were exposed to halogen bond-donors, resulting in a drastic change of the reflection. The systems were investigated in detail with respect to their optical, thermal and physical properties.

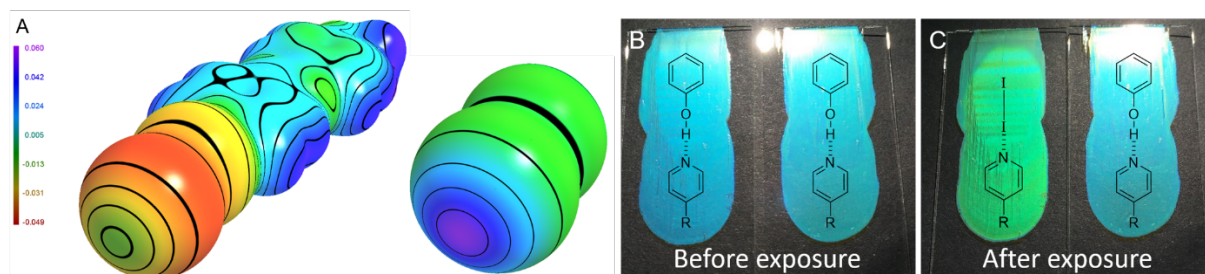


Fig. 1 a) Molecular electrostatic potential of an iodine-bond *pyridyl*-based complex (left) and the respective free iodine (right). b) and c) Demonstration of the structural colouration of a supramolecular liquid crystal at room temperature, caused by selective Bragg reflection, before and after exposure to halogen bond-donors.

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Properties of Natural Polyphenolic Compounds as Building Blocks for Supramolecular Liquid Crystals

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Polyphenolic compounds have shown their potential in the preparation of liquid crystalline materials. Their hydrogen-bond donating groups can be used in the design of supramolecular synthons to obtain LC materials.^[1]

The modular approach we used in this study aims to obtain supramolecular LC-materials, with tailored mesogenic properties and photoswitchability, out of natural obtainable compounds. Stilbenoids and chalconoids are a promising group of natural polyphenolic compounds. To investigate the structure property relationships of these supramolecular assemblies, the stilbenoids and chalconoids were chosen according to the position of their hydroxyl-groups.

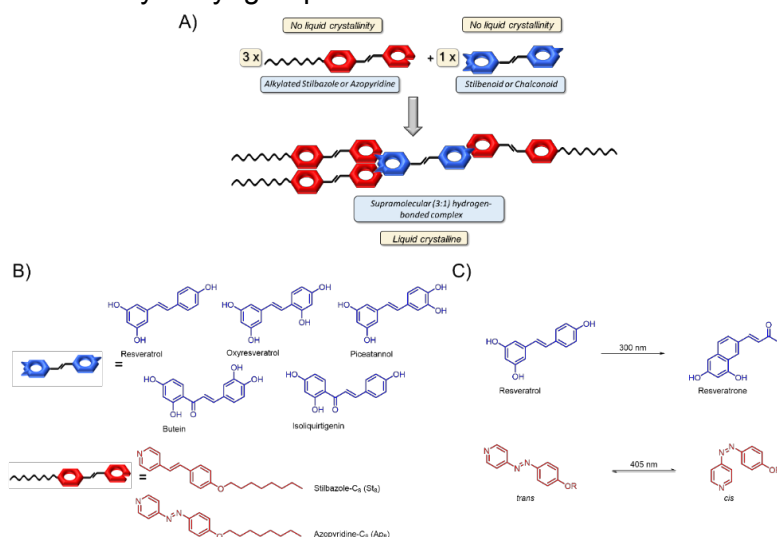


Fig 1 A) Schematic representation of the modular approach B) Molecular structure of the stilbenoids and chalconoids as hydrogen-bond donors (blue) and the alkylated stilbazoles and azopyridines as hydrogen-bond acceptors (red) C) photoswitchability of resveratrol and azopyridine.

As hydrogen-bond accepting moiety, azopyridines (**Ap**) and stilbazoles (**St**) are used. The addition of an azo compound introduces reversible photoswitchability into the system due to the photoinduced *cis-trans* isomerization of the azo-group. In addition to the *cis-trans* isomerization of **Ap**, the stilbenoid resveratrol can be transformed into resveratrone via a photochemical reaction.^[2] Thus, the combination of resveratrol with **Ap** enables selective dual-photoswitching by irradiation with UV-light.^[3]

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Stable-Radical Supermesogens for Potential Magnetic Applications

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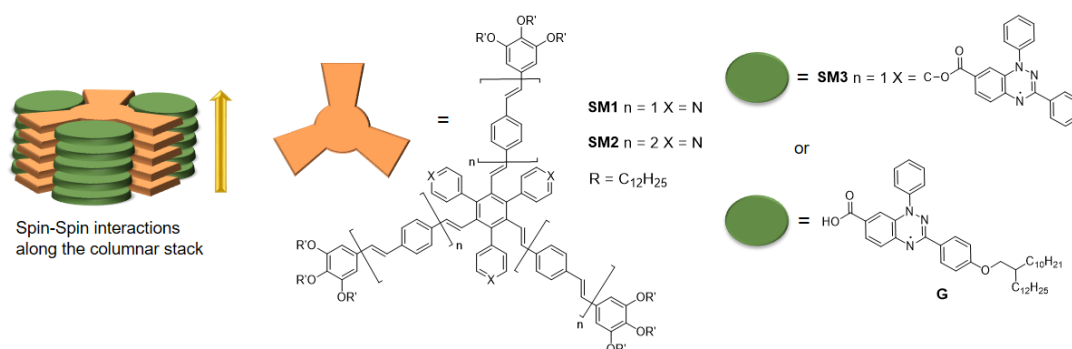


Figure 1. Proposed model of the double nanosegregated columnar stack. Structures of the host mesogens **SM1**, **SM2**, the guest blatter radical **G** and the covalent bound radical mesogen **SM3**.

Shape-persistent three arm star mesogens based on oligo(phenylenevinylene) (OPV) scaffolds provide void space between the conjugated arms, thus they can uptake up to three guest molecules via hydrogen bonding and function as endo-receptors.[1] These supramolecular supermesogens can arrange in a double nanosegregated structure when appropriate guest molecules are incorporated.[2] Such segmented columnar structures become highly attractive when functions are added to the different compartments. Such a function is paramagnetism induced with an organic stable radical. LC radicals were recently studied, with the aim to induce magnetic properties, such as shown in the emerging field covering magneto LC effects.[3] Therefore, Blatter radical derivatives have been introduced to **SM1-3** either by esterification or by hydrogen bonding (Figure 1), in order to investigate spin-spin interactions in the resulting columnar self-assemblies. The thermotropic properties of these stable radical mesogens were investigated by means of polarized optical microscopy (POM), differential scanning calorimetry (DSC) and X-ray scattering (XRS). The magnetic properties were studied by temperature variable EPR spectroscopy in the solid state. The results point to a change in the magnetic behavior of the material at the phase transition from the soft crystal to the liquid crystal. Similar observations have been recently described as “magneto-LC effects” in smectic liquid crystals containing a nitroxide radical group.[3]

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Tuning the solid-state emission of liquid crystalline nitro-cyanostilbene by Halogen Bonding

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The first observation of liquid crystalline mesophase in complexes formed via halogen bonded non covalent interaction using NO₂ as halogen acceptor has been reported and inspected systematically. The self-assembly properties of these complexes are sensitive to the type of the conjugation present in the building moieties and also the pattern of the peripheral alkoxy substitution. Non mesomorphic building blocks induced liquid crystallinity upon complexation whereas NO₂ building blocks having small mesophase range enhances the mesophase behaviour of the complexes. It has also been observed that with increasing chain length, wider mesophase range can be achieved. All the complexes are highly fluorescent in solid state whereas fluorescence disappeared upon melting or in solution state which shows AIEE effect in this complexes.

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Dielectric response of symmetric ether-linked cyanobiphenyl liquid crystal dimers

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Liquid crystal (LC) dimers are composed by two mesogenic groups, linked via a flexible spacer. Their physical properties and mesomorphic behaviour vary significantly compared to low molar mass mesogens and are highly dependent on the length and parity of the spacer. One of the most striking examples of such an odd - even effect is the observation of the Nx/tb phase in symmetric odd-membered LC dimers, which is absent in the corresponding even homologues [1]. The Nx/tb phase was initially discovered in odd-membered cyanobiphenyl methyl-linked dimers (CBnCB) [1], while the corresponding ether-linked CBO_nOCB dimers exhibit only the conventional N phase [2,3]. The only case, where Nx/tb phase is identified in CBO_nOCB dimers, is upon extensive supercooling of CBO₅OCB [3]. It is also notable, that odd members of the series are well-accommodated in the Nx/tb phase of binary mixtures between methyl- and ether-linked cyanobiphenyl dimers, where extensive stability and/or induction of the mesophase have emerged [4,5]. Within this work, the dielectric response of the symmetric cyanobiphenyl dimers of the 1,ω-bis(4-cyanobiphenyl-4',-yloxy)alkanes (CBO_nOCB) homologous series with odd number of carbon atoms in the flexible spacer ($n = 5, 7, 9, 11$) is extensively studied and compared to the dielectric response of the methyl-linked CBnCB dimers. The study is extended to selected binary mixtures of CBO_nOCB dimers along with Nx/tb forming CBnCB dimers. Interestingly, a non-typical behaviour in the temperature dependence of the parallel component of dielectric permittivity is observed in all members of the CBO_nOCB series, within the N phase. This behaviour is not related to any optical effect or to any non-typical electrooptic behaviour. The results are discussed in connection with the local intermolecular correlations [6], which are similar and present from the N phase in both methyl- and ether-linked dimers.

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Acknowledgement



The research work was supported by the Hellenic Foundation for Research and Innovation (HFRI) under the HFRI PhD Fellowship grant (Fellowship Number: 80996).

Molecular dynamics and crystallization behavior of liquid crystals in bulk and nanometric confinement

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Liquid crystals (LCs), as other molecular systems, can either vitrify or crystallize (melt crystallization) upon cooling. Liquid crystalline materials, have been also found to undergo so-called cold crystallization on heating from a glassy state. This talk will present the relaxation dynamics and kinetics of isothermal and non-isothermal crystallization processes in the nematic phase of two mesogenic fluorene derivatives (5P-EtFLEt-P5 [1] and 5P-Am*FLAm*P5 [2]), and contrasts them with the highly-ordered smectic B phase (SmB) of 4-n-butyloxybenzylidene-4'-n'-octylaniline (BBOA) [3,4]. The studies combines broadband dielectric spectroscopy (BDS), differential scanning calorimetry (DSC), and polarized optical microscopy (POM) measurements. It was revealed that 5P-EtFLEt-P5 and 5P-Am*FLAm*P5 display different types of non-isothermal cold crystallization. Our experimental results obtained for the crystallization process under isothermal conditions are discussed in terms of dynamic and thermodynamic properties of a material.

The second part of the talk will focus on the effect of confinement imposed by nanopores on the molecular dynamics and phase behavior of BBOA liquid crystal [5]. The phase transition temperatures of bulk BBOA and enclosed in napores show linear dependence as a function of inverse pore diameter. The BDS investigations revealed new relaxation processes associated with gradual paranematic-to-nematic transition in nanopores. Special emphasis is given to the influence of geometrical restriction on the non-isothermal crystallization process upon cooling. Finally, the impact of spatial constraint on intramolecular vibrations of alkyl chains in the course of crystallization will be discussed in the context of Fourier transform-infrared spectral data.

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This work was financially supported by a National Science Centre (Grant SONATA11: UMO-2016/21/D/ST3/01299).

Superior electro-optic response in Organic N-benzyl-2-methyl-4-nitroaniline doped in nematic liquid crystal device

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Abstract: A superior electro-optical response has been achieved by doping organic N-benzyl-2-methyl-4-nitroaniline (BNA) in nematic liquid crystals (LCs) reported in this study. The BNA-doped LC cells have a fall time that is fivefold faster than the pristine LC cell. The possible reason behind the fall time could be the remarkable decrements in the rotational viscosity and threshold voltage by 45% and 27%, respectively, and the strong additional restoring force resulted from the spontaneous polarization electric field of BNA. On the other hand, the BNA doped LC has the dielectric anisotropy ($\Delta\epsilon$) of the LC mixture is increased by 7%. Furthermore, the BNA doping reduces the phase transition temperature, birefringence, order parameter, and splay elastic constant of the LC mixture but enhances the $\Delta\epsilon$ of the LC mixture. The phenomena bring out that organic doping decreases the threshold voltage of the LC cell. Density functional theory (DFT) theory calculation demonstrates that the BNA dopant causes a strong absorbance in the near wavelength of 400 nm; decreases the molecular energy gap, increased dipole moment, polarizability, and polarizability anisotropy hence increase the $\Delta\epsilon$ of the LC mixture, which well agrees with the experimental results. BNA doping has appropriate to fabricate a fast response and strong absorbances for ultraviolet (UV) light, potentially anti-UV applications, such as anti-UV smart windows, glasses, and promising application fields of LC devices and displays.

Keywords: Organic molecule; N-benzyl-2-methyl-4-nitroaniline (BNA); liquid crystal; fast response time; density functional theory(DFT).

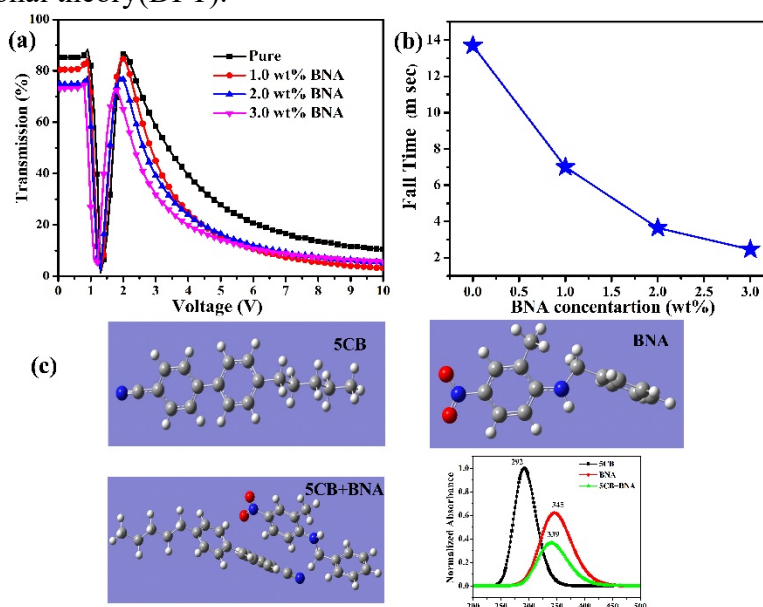


Figure. (a) V–T curves (b) fall time of the BNA-doped LC cells and (c) Optimized geometry structures and theoretical absorption spectra for BNA, 5CB, and BNA+5CB using DFT (Gaussian 09).

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Synergistic structures in lyotropic lamellar gels

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Gelled lyotropic liquid crystals are soft materials which combine the anisotropy of a lyotropic liquid crystal with the mechanical stability of a physical gel [1]. In this contribution we will present the results of small-angle neutron (SANS) and X-ray (SAXS) scattering studies which show that synergistic structures, which neither exist in the non-gelled L_α phase nor in the isotropic binary gel are formed in the lamellar gels in cases where the fiber diameter considerably exceeds the lamellar repeat unit.

A lamellar L_α phase was gelled using the two low molecular weight organogelators 1,3:2,4-dibenzylidene-D-sorbitol (DBS) and 12-hydroxyoctadecanoic acid (12-HOA). In the case of DBS the thickness of the gel fibers is in the same range as the lamellar repeat distance of the L_α phase. In the case of 12-HOA however, the gel fiber diameter exceeds the lamellar repeat unit several times. In this case, the SANS curve of the gelled L_α phase shows a pronounced shoulder at $q \approx 0.02 \text{ \AA}^{-1}$, which is not present in the curves of neither the non-gelled L_α phase nor the binary gel (see Fig. 1a). Additionally, the 2D X-ray diffraction pattern of the gelled L_α phase (Fig 1b) demonstrates that most of the fibers are aligned along the layers instead of the fibers running arbitrarily through the anisotropic solvent. These results can be quantitatively explained by synergistic structures such as the one shown in Fig. 1c, where the lamellar layers are wrapped around the fibers to avoid the formation of topological defects. Interestingly, such structures mimic similar schemes found in neural cells, where axons are surrounded by lamellar myelin sheets. Contrary, in the case of the thin DBS fibers no indication for a formation of synergistic structures was found [2]. We will discuss the SANS data evaluation model, the synergistic structures derived thereof and the reasons behind the formation of synergistic structures.

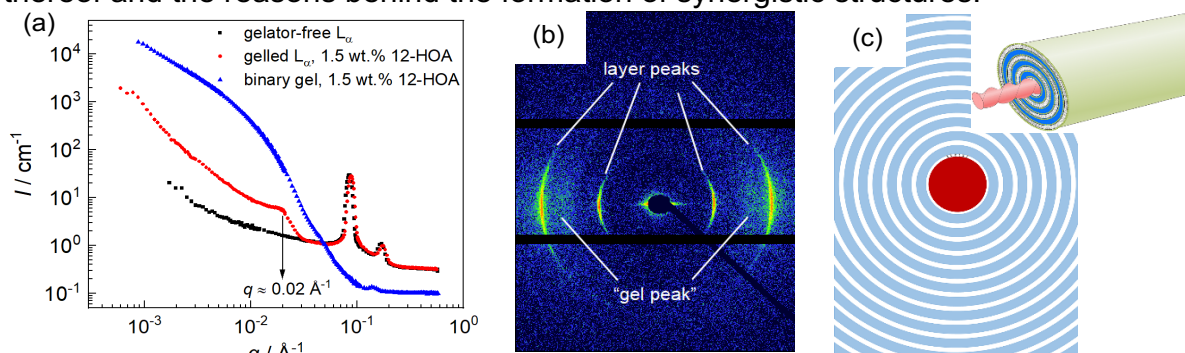


Figure 1: (a) SANS curves of the 12HOA-gelled L_α phase (red), the corresponding non-gelled L_α phase (black) and the binary gel n -dodecane/12-HOA (blue). (b) 2D X-ray diffraction pattern of the L_α phase gelled with 12-HOA. (c) scheme of a synergistic lamellar gel structure formed in the case of thick fibers.

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Acknowledgement: The authors gratefully acknowledge financial support from the *Deutsche Forschungsgemeinschaft* (DFG Gi 243/9-1 and Gi 243/9-2) and *Fonds der Chemischen Industrie* (FCI). We thank Ralf Schweins and Sylvain Prévost for their help with the SANS experiments at the Institut Laue-Langevin (ILL) in Grenoble, France and Prof. Thomas Hellweg and Carina Dargel for the 2D SAXS experiments.

Deformed lying helix transition in cholesteric LC layers at spatially periodic boundary conditions

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/The field-induced orientational transition in layers of cholesteric liquid crystals with spatially periodic modulation of the surface anchoring is studied by numerical simulations and experimentally [1]. The modulation of the surface anchoring is implemented using high-resolution focused ion-beam treatment of a polymer film providing planar alignment conditions. A specific feature of the orientational transition is that the thermodynamically stable initial planar structure with the helix axis along the normal to the layer transforms under an electric field into an equilibrium structure with a deformed lying helix (DLH) in the plane of the layer. For such a transition to occur the natural pitch of the cholesteric helix must be substantially less than the anchoring modulation period. The appearance of the DLH with a pitch corresponding to the anchoring modulation period results in strongly enhanced first-order diffraction efficiency. The orientational DLH transition is characterised by a rather narrow driving voltage range with a pronounced hysteresis. The waveguide lasing effect with characteristic of the deformed helix spectral modes is demonstrated in a range of the DLH transition.

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Generalized Landau-de Gennes theory of the twist-bend nematic phase: on the role of flexopolarization

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Twist-bend nematic (N_{TB}) is a novel liquid crystalline phase, which existence has been unequivocally confirmed less than eight years ago [1, 2]. It forms through the unique phenomenon of spontaneous chiral symmetry breaking in the liquid crystalline system of achiral bent-shaped molecules. To the set of uncommon properties of this phase, one can add: heliconal structure of a nanoscale pitch without long-range positional order of molecules and a degenerate sign of the chirality (ambidextrous chirality). These features ignited a worldwide interest in N_{TB} , which pushed it to the forefront of hot topics in liquid crystal research [3].

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 $P_\alpha(\mathbf{r})$ [4-6]. 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.e. 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 remaining 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 [7].

Acknowledgments: This work was supported by Grant No. DEC-2013/11/B/ST3/04247 of the National Science Centre in Poland. LL acknowledges partial support by the EPSRC grant EP/R014604/1 [The Mathematical Design of New Materials] of the Isaac Newton Institute for Mathematical Sciences, University of Cambridge, UK. WT acknowledges partial support by Marian Smoluchowski Scholarship (KNOW/58/SS/WT/2016) from Marian Smoluchowski Cracow Scientific Consortium "Matter-Energy-Future" within the KNOW grant and by Jagiellonian Interdisciplinary PhD Programme co-financed from the European Union funds under the European Social Fund (POWR.03.05.00-00-Z309/17-00).

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Photosensitive Fluorinated Hydrogen-Bonded polycatenars

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Azobenzene-based liquid crystals (LCs) whose properties could be modified with UV-visible light irradiation are of great interest for photosensitive and photoswitching materials [1]. Noncovalent interactions such as hydrogen or halogen bonding are very useful for obtaining LCs with complex superstructures via easily accessible synthetic pathways. We have reported recently the first examples of light-responsive halogen bonded as well as hydrogen-bonded supramolecular polycatenar LCs [2,3]. The hydrogen-bonded LCs were able chiral isotropic liquid phase (Iso₁^[*]) beside chiral cubic phases (Cub^[*]) [3]. Herein we report about the effect of the lateral fluorination at different positions in the molecular structure of these H-bonded LCs on their liquid crystalline behaviour (**Figure 1**). The new supramolecules were constructed via intermolecular hydrogen bond formation between fluorinated azopyridine derivatives and benzoic acid derivatives. The liquid crystalline behaviour was investigated in detail by differential scanning calorimetry (DSC), polarized optical microscope (POM) and X-ray diffraction (XRD). Depending on the position of the fluorine atom different types of LC phases were observed including Iso₁^[*], Cub^[*], achiral cubic in addition to tetragonal phases. This report proves the potential of fluorination as a powerful tool for the modifications of the LC behaviour of the supramolecular materials.

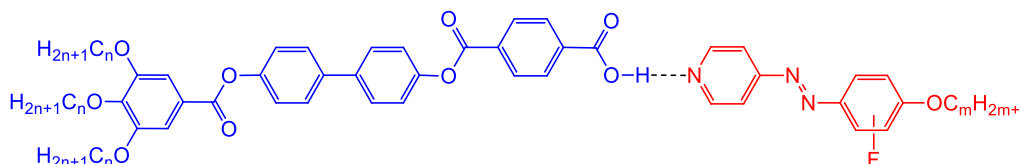


Figure 1. Chemical structures for the supramolecular LCs under discussion.

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Characterisation of strongly fluorescent mesogens with quinoxaline based cores

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Quinoxaline derivatives with mesogenic properties were synthesized and studied. Majority of compounds form a columnar hexagonal Col_h phase, containing one molecule for column cross section. Some of the studied materials in temperature range below Col_h phase exhibit another columnar structure, with crystallographic unit cell being distinctly larger. Studied compounds exhibit strong fluorescent properties, some of them show large Stokes shift (about 50 nm), that suggested strong molecular π - π interactions along the columns. Modification of molecular structure of the compounds could easily change the fluorescent properties; additional terminal chains or condensation of benzyl rings within quinoxaline unit caused the significant shift of the absorption/fluorescence wavelength. Synthesized materials could be easily aligned in Col_h phase which permitted to measure the anisotropy of hole conductivity in this phase. The suitability of new materials for preparing organic field transistors was tested.

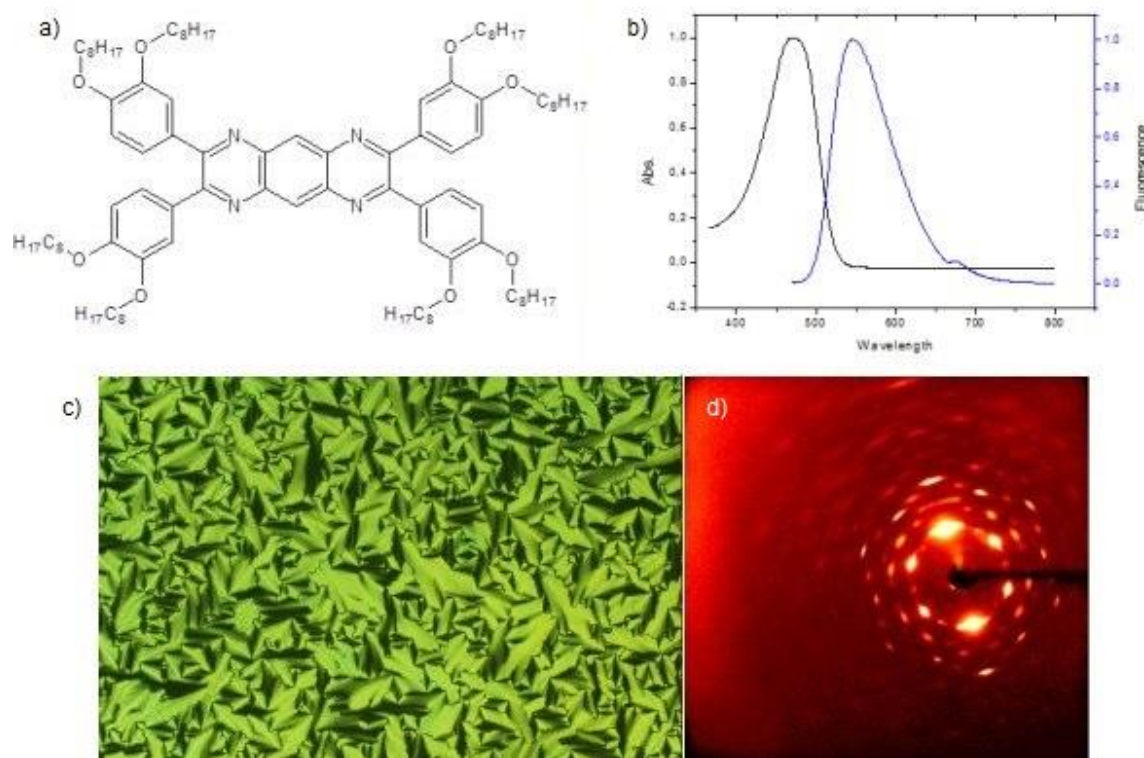


Figure 1 – Molecular structure of one of the studied compounds (a), its absorption and fluorescence spectra (b), optical texture of Col_h phase (c) and x-ray diffraction pattern of low temperature columnar phase (d).

Modeling of self-organizing photonic structures

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Nematic liquid crystals doped with gold nanoparticles are used in various photonic systems. Depending on the type of nanoparticles (metallic, ferroelectric, dielectric, etc.), their size, shape, concentration or surface coating, liquid crystals doped with nanoparticles may exhibit different properties [1–4]. Metallic nanoparticles show great promise in device applications due to their ability to improve liquid crystal performance. An interesting effect in such a composite is the spontaneous formation of the photonic structure observed two years ago [5]. The spontaneous pattern formation observed in the experiment can be mimicked and reproduced in the formalism of diffusion-reaction systems. Formalism was introduced by Alan Turing in 1952 [6] to explain the phenomenon of morphogenesis. His approach was later successfully applied to generate patterns found on shells, fish, zebras, leopards, giraffes, etc. In such systems, two agents or chemicals (activator and inhibitor) interact and dissipate. These interactions can be viewed as functions applied to actual concentrations, determined by a nonlinear partial differential equation. If the diffusion rates of the two chemicals are not equal, the initially well-mixed, homogeneous concentration state of the chemicals can lead to spatially inhomogeneous patterns such as stains or stripes. In the context of the optical experiment discussed in the presentation [5], gold nanoparticles play the role of an activator. Their number decreases in an autocatalytic process, in which the isotropic domain slowly spreads, repelling gold nanoparticles, and reducing the amount of these nanoparticles automatically forces the domain to grow. Repulsed gold nanoparticles concentrate in separated areas and by increasing the critical temperature of the transition from the nematic to isotropic phase, they reduce the likelihood of an isotropic phase in these areas, and thus have an inhibitory effect.

- [1] T. Hegmann, et al., *J. Inorg. Organomet. Polym. Mater.* 17 (3) (2007) 483–508.
- [2] O. Stamatoiu, et al., in: C. Tschierske (Ed.), *Liq. Cryst. Top. Curr. Chem.*, vol. 318, Springer, Berlin, Heidelberg, 2011.
- [3] U. Shivakumar, et al., *Liq. Cryst.* 38 (11–12) (2011) 1495–1514.
- [4] S. Orlandi, et al., *Phys. Chem. Chem. Phys.* 18 (2016) 2428–2441. [5] S.K. Prasad, K.L. Sandhya, G.G. Nair, U.S. Hiremath, C.V. Yelamaggad,
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Particle size dependent phenomena in lyotropic graphene oxide liquid crystals

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Graphene oxide (GO) flakes are disk-shaped colloidal particles, the thickness of which is just a few atomic layers and thus on the molecular length scale. Their lateral dimensions however are on the colloidal length scale and can vary from several microns down to some ten nanometers (Fig. 1b). As a result of their high steric anisometry, lyotropic nematic liquid crystals (LC) are formed in water without any further additives at remarkably low concentrations below 0.1 wt% of GO (Fig. 1a) [1,2]. This extremely low GO content however seriously complicates the investigation of these phases by classical methods of LC science such as DSC or X-ray scattering.

In this contribution we will present a new procedure to obtain GO-LCs with specific and narrow-distributed lateral dimensions of the GO building blocks ranging from about 60 nm to 4 μm . We will also discuss the results of recent experiments, including sedimentation, light scattering and Kerr effect measurements, and show that the size of the GO building blocks has strong impact on many LC properties, such as the diffusion and sedimentation behavior, the textures and the phase diagrams of GO-LCs. For instance, nematic LCs of micron-sized GO-flakes form large-scale *schlieren* textures which can be easily seen by the naked eye (Fig 1a) and which appear grainy under the microscope (Fig 1b), similar to the textures of mineral LCs [3]. In the case of nano-sized GO flakes however the typical *schlieren* texture of micellar or low-molecular nematic LCs (Fig 1b) are observed. In conclusion, in GO-LCs the dimensions of LC building blocks can be varied in a controlled way over several orders of magnitude. In this sense GO-LCs bridge the gap between mineral LCs formed by micron-sized colloidal particles and lyotropic LCs formed by nanometer-sized micelles.

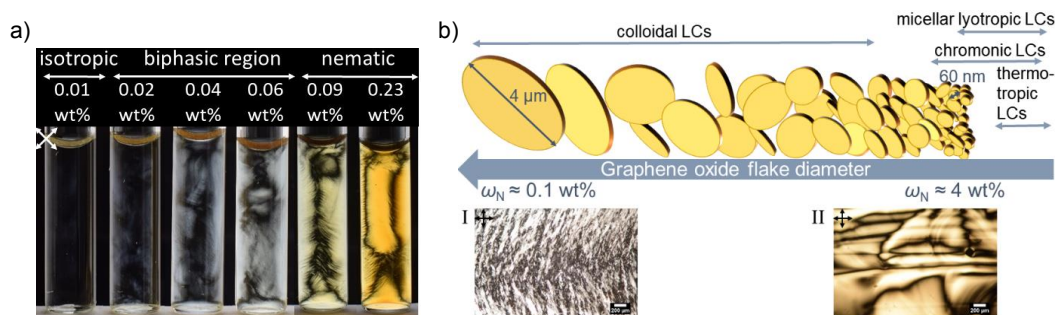


Fig. 1: (a) Images of colloidal graphene oxide (GO) liquid crystals (flake diameter $\approx 4 \mu\text{m}$) showing the isotropic to nematic phase transition in the GO concentration range of 0.01 – 0.23 wt% in pure water. (b) Dimensions of GO flakes compared to the dimensions of building blocks in other classes of LCs. With decreasing flake size, the weight fraction ω_N of the nematic phase formation is shifted towards higher concentrations and the corresponding schlieren textures (I, II) smooth out.

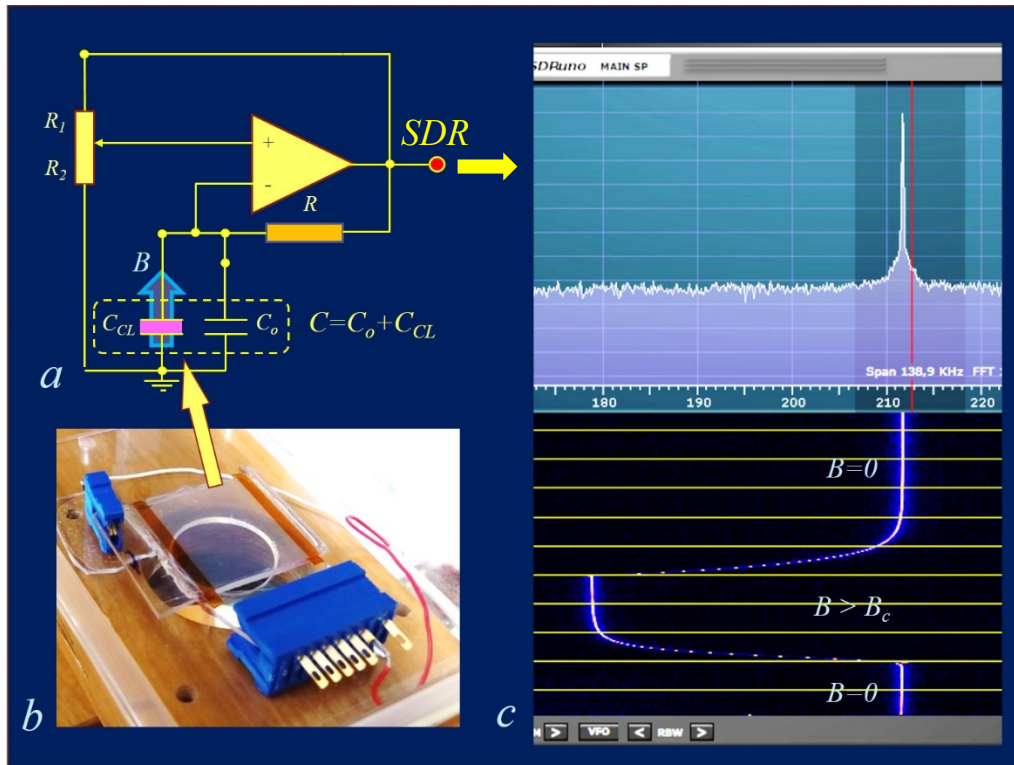
- [1] J. E. Kim et al., *Angew. Chem. Int. Ed.*, **50**, 3043-3047, (2011).
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Fréedericksz transition On Air

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Setup: a) Op-amp RC oscillator, b) TND used as a condenser, c) application of the magnetic field B results in a shift of the oscillation frequency detected and made audible with a radio (SDR) in DSB mode.

In 1924, M. Jeżewski [1] and W. Kast [2] discovered the dielectric anisotropy of nematic PAA using LC resonant circuits in which the condenser C was filled with PAA. Upon application of a magnetic field orthogonal to the condenser's electrodes, they measured frequency shifts corresponding to changes in the permittivity ϵ of PAA. In the spirit of this epoch, they interpreted these results as due to orientation of molecular swarms by the magnetic field. Three years later, Fréedericksz and Repieva [3] interpreted the action of the magnetic field on nematics in terms of the long-range elasticity of nematics.

We built a modern version of the Jeżewski-Kast setup (see the figure) which is simple enough to be used as a class-room experiment. We used a Software Defined Radio (SDR) operating in the Double Side Band mode which makes the field-induced frequency shifts audible. This setup is astonishingly sensitive and allows to measure all static and dynamic characteristics of the Fréedericksz transition [4].

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Short Talks and Posters

Spatially localized electrooptical modes in vertically aligned nematic LCs

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Electrooptical switching and liquid crystal (LC) director distribution have been studied in spatially periodic electric field for vertically aligned nematic LCs with both negative [1] and positive dielectric anisotropy [2, 3]. The electric field has been created using interdigitated electrodes of a period less than $3\ \mu\text{m}$. We found that if the thickness of LC cell is smaller than the period of electrode structures the fast near-to-surface director reorientation gives main contribution to electrooptics. The electrooptical switching is accompanied with the appearance of domain walls stretching across the cell. They divide a volume of LC into domains and speed up the relaxation process.

The 3D-numerical simulation (fig.1a, b) shows very good agreement with the experimental results: for LC with positive dielectric anisotropy the fast and slow modes of deformation are found, while for LC with negative dielectric anisotropy two fast optically distinguished modes are observed.

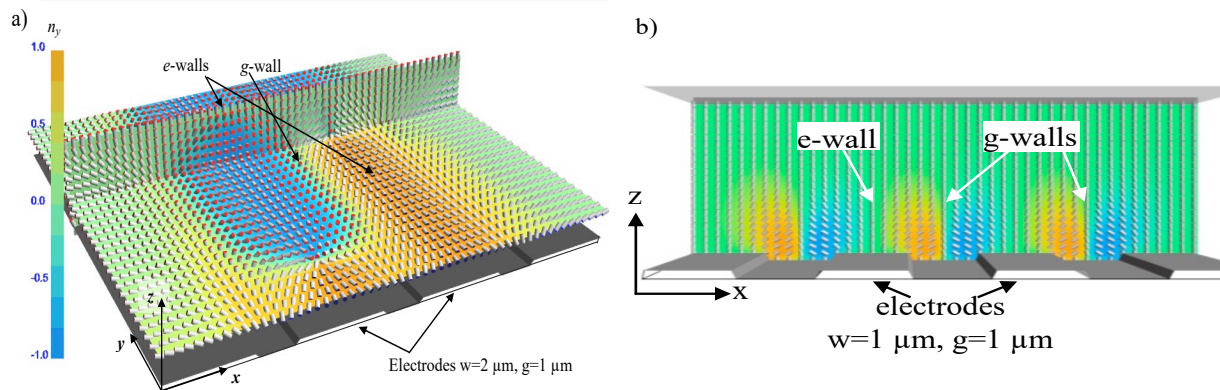


Figure 1. Calculated LC director distribution for the spatial domain of LC with negative (a) and positive (b) dielectric anisotropy. The color corresponds to n_y component (along electrode stripes) of the LC director. Electrode (e-) and gap (g-) walls are related to the domain walls above and between electrodes stripes.

Acknowledgements: This work has been supported by the Ministry of Science and Higher Education of Russian Federation within state assignment to FSRC “Crystallography and Photonics” RAS.

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Coalescence of liquid droplets in a quasi 2D liquid film

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Coalescence of liquid droplets is an important phenomena in biological, chemical and physical systems as well as in modern technology. Various experimental and theoretical studies explored droplet dynamics in 3D and on 2D solid or liquid substrates [1-3]. Here, we demonstrate coalescence of isotropic droplets in thin quasi 2D liquids, an overheated smectic A films. Close to the SmA-Iso transition temperature the inner layers of the film start to melt while the outer layers stay in the SmA phase. The isotropic material then forms flat liquid droplets. We investigated their dynamics experimentally and measured the shape deformation during the whole merging process using high-speed imaging. We used monochromatic light to visualize interference fringes to reconstruct the complete height profile. This droplet coalescence in a quasi 2D liquid film is a unique example, where the lubrication approximation can be directly applied, and the smectic membrane plays the role of the precursor film. Our studies reveal the scaling laws of the coalescence time depending on the droplet size and the material parameters. We also compared our results with existing models for liquid lens coalescence on liquid and solid surfaces. FEM simulation also verify the lubrication approximation for our system.

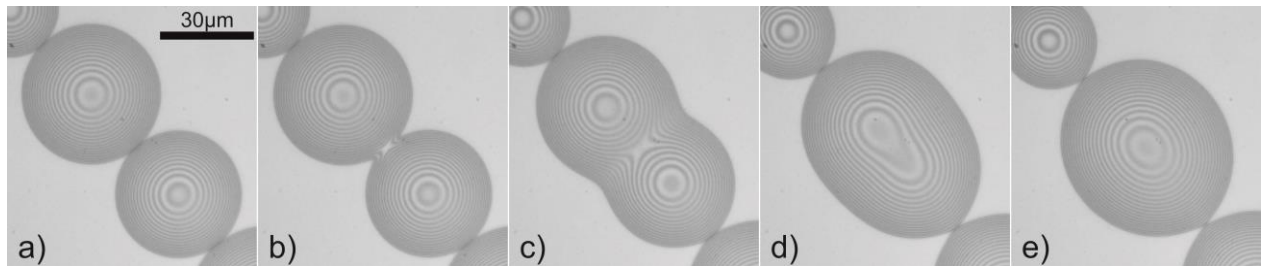


Fig. 1: Top view of two merging droplets with interference fringes in monochromatic light at time a) $t=0\text{ms}$, b) $t=0.25\text{ms}$, c) $t=0.75\text{ms}$, d) $t=1.25\text{ms}$ and e) $t=1.75\text{ms}$, the initial droplet diameters are $D_1=35.5\mu\text{m}$, $D_2=34.7\mu\text{m}$ with the initial height of $H_1=1.13\mu\text{m}$, $H_2=1.10\mu\text{m}$

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Electro-optical addressing of meta-surface based optical tweezers

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Optical tweezers are well-established tools to investigate dielectric microparticles. By focusing or defocusing a laser beam, particles can be trapped or released, respectively [1]. The target of our research is to develop a lens for this purpose that can be switched between a focusing and a defocusing state by applying a voltage. Instead of a microscope lens, we use a geometric phase array which acts as a convex lens for right-handed circularly polarized (RCP) light and as a concave lens for left-handed circularly polarized (LCP) light. A liquid crystal (LC) cell is applied to switch the state of polarization of the light from LCP to RCP.

The phase object which serves as a lens is a two-dimensional array of silicon nano-antennas (Pancharatnam-Berry meta-surface) [2]. Each antenna has a height of 600 nm, a length of 200 nm and a width of 120 nm (**Fig. 1**). The circular array has a diameter of 800 μm and is designed for light with a wavelength of 800 nm. The resulting focal length is 530 μm and the numerical aperture is 0.6.

The electro-optic LC cell can switch between RCP and LCP light at a wavelength of 800 nm, so that we can selectively focus or defocus the light transmitted through the meta-lens, thereby trapping particles or releasing the microparticles from the optical trap, respectively.

The cell consists of two layers, an active twisted nematic (TN) LC cell and a passive quarter-wave-plate (QWP) (**Fig 2**). The TN-cell is filled with the LC mixture E7 (Merck) and the QWP is a polymer-film prepared from a mixture of the photoreactive LC-monomer RM257 (Synthon) and E7. Similar devices were built in previous studies [3], but the manufacturing conditions have to be tuned for the wavelength of 800 nm. To get the right manufacturing conditions, we investigate the influences of different parameters for fabricating the QWP: the thickness, the ratio of the components and the polymerization temperature. Optimizing these parameters is facilitated by analyzing the Stokes parameters of the light transmitted through the layers.

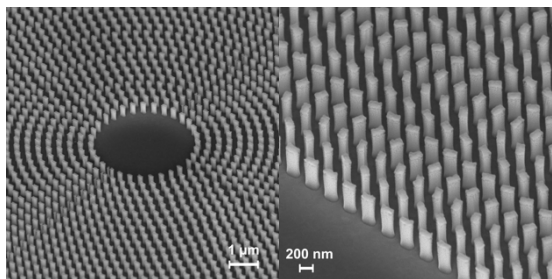


Figure 1: SEM images of the meta-lens.

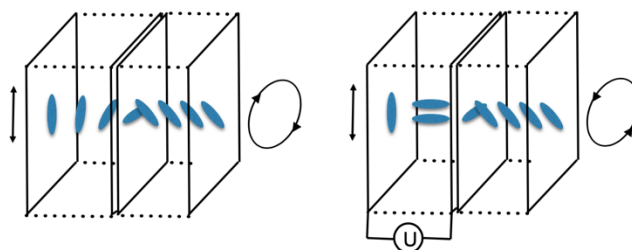


Figure 2: Principle of the electro-optic switch.

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Cholesteric Ring Resonators

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It is a well-established fact that cholesteric liquid crystals (CLCs) show resonant optical modes at the two edges of the selective reflection band. These resonances have been used in thin-film geometries for the generation of laser emission. In a theoretical treatment, the properties of cholesteric ring resonators are discussed, where the light propagates along a circular path in a cholesteric medium.

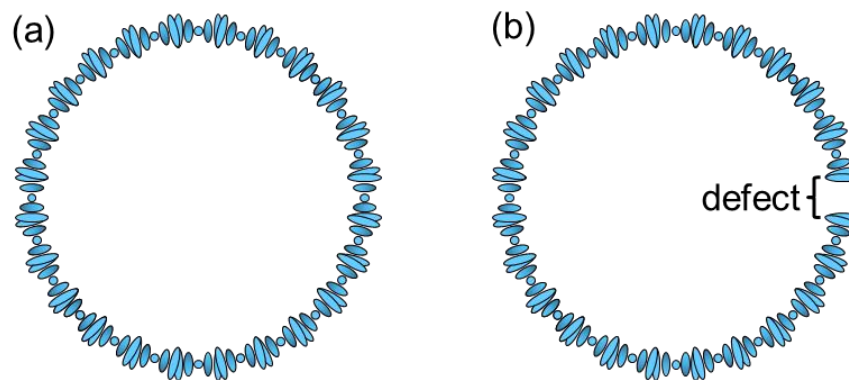


Figure 1: Sketches of cholesteric ring resonators – without defect (a), and with a defect layer interrupting the cholesteric helix (b).

Apart from the band-edge resonances (originating from the periodicity of the CLC), in a cholesteric ring resonator (Fig. 1a) there exist additional resonant modes due to the confinement of the light in the ring cavity. In the vicinity of the reflection band, the non-linear dispersion of the CLC's eigenmodes strongly affects the frequency spacing of these resonances.

An artificial defect in the cholesteric helix (like an optically isotropic defect layer, a discontinuity of the director orientation, or a combination of both) gives rise to additional resonant modes, localized at the position of the defect. Such photonic defect modes have been widely studied in thin-film geometries, and can be used for the realization of narrow-band optical filters and for the generation of low-threshold laser emission. Incorporation of such structural defects in a cholesteric ring resonator (Fig. 1b) results in a coupling of the CLC's eigenmodes, and strongly affects the frequencies and polarization properties of the resonant modes of the ring cavity. The resonator properties can be finely tuned by adjusting the defect geometry.

Possible experimental realizations of such cholesteric ring resonators will be discussed, as well as potential applications (e.g. for optical sensing).

Polymer Dispersed Liquid Crystal Films Doped with Carbon Nanotubes: Modeling of the Electrooptical Response

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Polymer Dispersed Liquid Crystals (PDLC) are composite materials consisting of small liquid crystal (LC) droplets surrounded by a polymer matrix. Due to their relatively easy preparation and processing, the PDLC devices found many applications such as displays, architectural windows, energy control devices, projection displays, spatial light modulators, polarizers. Carbon nanotubes (CNTs) have excellent mobility and electrical conductivity, thus being suitable as doping nanoparticles (NPs) in order to improve the electrically - controlled orientation of LC.

In this work the optical model has been developed for analyzing the coherent (regular, direct) transmittance of a polymer dispersed liquid crystal films doped with carbon nanotubes [1]. It is based on the Foldy–Twersky and anomalous diffraction approximations, Maxwell-Garnett equations, and the order parameters concept. The model allows one to analyze the electro-optical response of films depending on the film thickness, the refractive indices of the liquid crystal (LC) and the polymer matrix, the size and concentration of the LC droplets, the concentration of nanotubes, the dielectric permittivities of the LC, the polymer and the nanotubes.

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The “Click-Procedure” extended to Porphyrin Star Mesogens?

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In recent years porphyrins have been successfully applied in organic electronic and especially in photovoltaics (OPV) [1]. Even porphyrin-fullerene dyads have been claimed as liquid-crystalline OPV additives. Unconventional star mesogens consisting of a phthalocyanine core and a linear oligo(phenylenevinylene) scaffold around the core possess intrinsic free voids between the shape-persistent arms, which can host fullerenes via a newly discovered Click process [2]. In the present contribution an analogous system is developed, in which the core is exchanged with Zinc-porphyrin and the arms by oligo(thienyl) scaffolds [3].

Zinc-porphyrins, with conjugated arms at the *meso*-positions are robust molecules and in contrast to the regioisomeric phthalocyanines highly symmetric. Consequently, the Click-process between a space providing mesogen **1** (X = H) and a sterically overcrowded derivative **2** (X = Ful) (Figure 1) is expected to yield a triple nanosegregated assembly, in which porphyrins are locked to the columnar centre in π -stacks, fullerenes are nanosegregated in helical strands around the column and the conjugated scaffolds acts as antenna system in between these building blocks. This work will highlight the optimised synthesis towards the target materials. The LC properties and structure of the neat compounds and the 1 : 1 mixtures of **1** and **2** will be studied by polarized optical microscopy, differential scanning calorimetry and comprehensive X-ray scattering. We aim to discover a liquid crystal with an ideal donor-acceptor nanosegregated system as future bulk heterojunction material, which can be applied in OPVs or photosensitive transistors by using the appropriate length of the conjugated arms (n, m), spacer lengths (o) and peripheral chains (R).

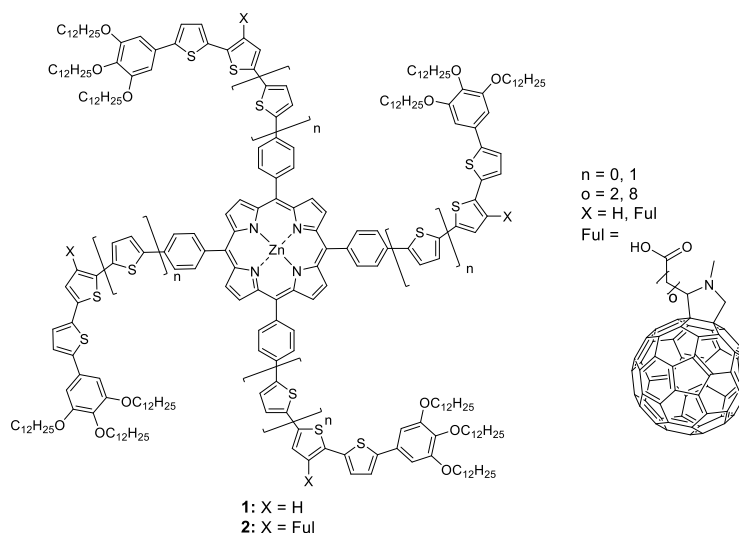


Fig. 1: Star-shaped, shape-persistent target molecules.

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Design and synthesis of liquid-crystalline dimers exhibiting B₄ phase

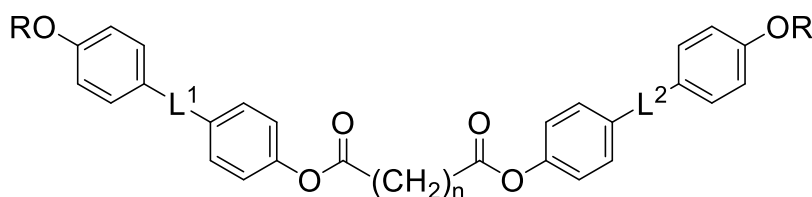
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¹Department of Organic Chemistry, University of Chemistry and Technology Prague, 16628 Prague

²Institute of Physics, Academy of Sciences of the Czech Republic, 182 21 Prague

In the last decade of twentieth century, liquid crystals formed by bent-core molecules opened up an exciting new area of research exploring a large number of intricately structured mesophases. Smectic arrangement of achiral bent-shaped materials often tends to exhibit a spontaneous breaking of reflection symmetry and formation of chirality-segregated domains. They occur in phases such as the dark conglomerate or B₄ phase.

Hereby, we present molecular design, synthesis and characterization of liquid-crystalline dimers based on glutaric and pimelic acid. We have introduced various building blocks into the molecular structure, such as a photoresponsive azobenzene unit, aromatic side arms containing an ester linking unit as well as terminal alkyl chains of different length, in order to study their influence on B₄ phase formation and the value of melting point (Figure 1).



I: $n = 3$, $L^1 = \text{N}=\text{N}$, $L^2 = \text{N}=\text{N}$	R: a = C ₈ H ₁₆ ,
II: $n = 3$, $L^1 = \text{OOC}$, $L^2 = \text{COO}$	b = C ₁₁ H ₂₃
III: $n = 5$, $L^1 = \text{N}=\text{N}$, $L^2 = \text{N}=\text{N}$	c = C ₁₆ H ₃₃
IV: $n = 5$, $L^1 = \text{OOC}$, $L^2 = \text{COO}$	

Figure 1: Structure of prepared materials

This work was supported by the Czech Science foundation (reg. No. 19-03564S).

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Influence of single-walled carbon nanotubes and liquid crystal 5CB admixtures on physical properties of L,D-PLA

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Ecological solutions are becoming more and more popular every year in many areas of life, which causes an increase in demand for new functional materials for use in modern environmentally friendly electronic devices [1,2]. To meet these requirements, we have created flexible hybrid layers based on biodegradable polymer L,D-poly(lactic acid) (L,D-PLA) with an admixture of conductive single-walled carbon nanotubes (SWCN) and liquid crystal 4'-pentyl-4-biphenylcarbonitrile (5CB), in various ratios by weight [3]. New created hybrid materials were investigated by polarizing microscopy method to find the difference in the morphology. Especially, the changes were observed for the layers with a larger 5CB admixture. The dielectric spectroscopy and two-probe methods were used to determine the electric properties of new hybrid layers. We showed that addition of 5CB with ratio 1:10 improves both the flexibility and the conductivity of the hybrid layers based on SWCN and L,D-PLA. Thermal stability of the created hybrid layers was studied by differential scanning calorimetry method.

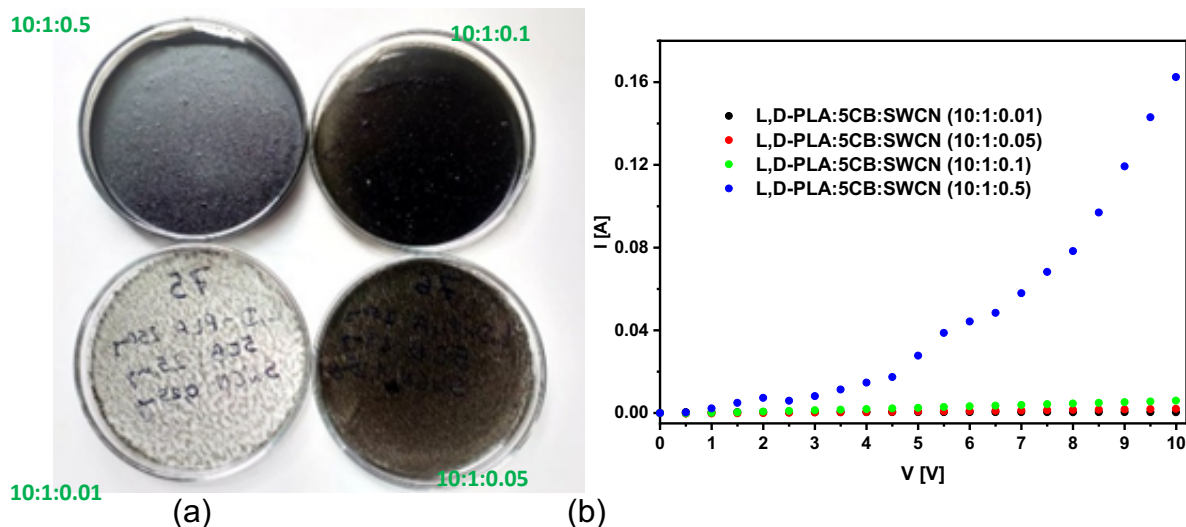


Figure 1 Photo of created layers in different weight ratio (a) and current-voltage characteristics (b) for created layers based on L,D-PLA, 5CB and SWCN [3].

- [1] T. Someya, et al., *Nature*, **540**, 7633 (2016).
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- [3] P. Fryń, et. al., *Polymers*, **11** (11),1867 (2019).

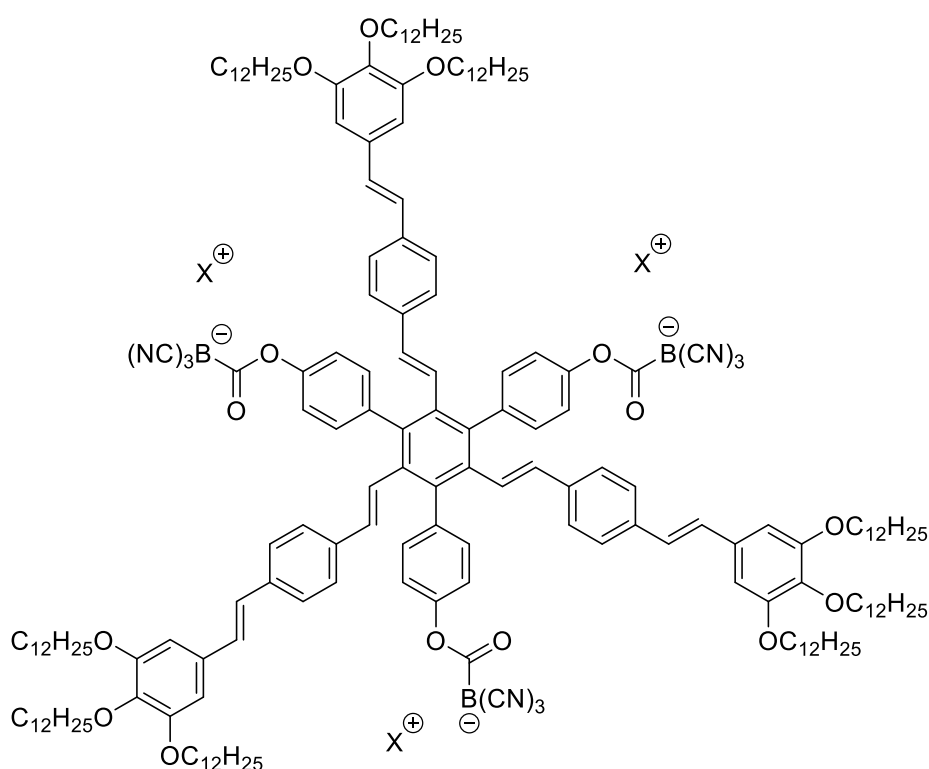
Controlling the Liquid-Crystalline Phase by Ionic Guests

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Hexasubstituted C_3 -symmetric star shaped molecules with a benzene core and oligo(phenylenevinylene) arms form columnar liquid crystals (LC) with cavities [1]. These cavities can be filled with guest or pseudo guest molecules in order to functionalize the star mesogen [2]. Aim of this project is to covalently link ionic monocarboxy cyanoborates [3] via esterification reaction to produce oriented ion channels. A point of interest hereby is the variation of the counter ions and resulting changes in the structure and stability of the liquid crystalline phase. These molecules could be used as ion conducting membranes, e.g. in dye sensitized solar cells or fuel cells.

The ionic star mesogenes are studied by polarized optical microscopy, differential scanning calorimetry and comprehensive X-ray scattering, helping to understand the structure-property relationship of these liquid-crystalline phases in order to optimise the material for future applications.



$X = \text{NnBu}_4; [\text{K}[18]\text{crown-6}]$

Fig. 1: Hexasubstituted C_3 -symmetric star shaped molecules with different ionic moieties.

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Understanding the phase behavior of ionic liquid crystals: the role of the charge position – A simulation study

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Ionic liquid crystals (ILCs) combine anisotropic with ionic features and this makes them interesting for various applications. One key property is the highly anisotropic charge transport in ILCs [1,2]. In order to rationally design ILCs the relationship between phase behavior and structure has to be understood. The most common liquid crystalline phases in ILCs are smectic A phases while nematic phases are extremely rare [2]. To better understand this the authors of Ref. [3] used density functional theory and showed that the location of the charge on the mesogen seems to fundamentally influence the phase behavior. In their case the nematic phase only occurs when the charge is positioned at the center of the mesogen. However, detailed knowledge about the influence of the charge position on the presence or absence of a nematic phase in ILCs is still lacking.

Here we present a simulation study of 1:1 mixtures of rod-like Gay-Berne (GB) and spherical Lennard-Jones (LJ) particles of opposite charge. The cation of the ILC is represented by a GB particle and the anion is modeled by a LJ particle. We vary the position of the charge on the GB particle (see Figure 1a) from its center to its tip in different simulation runs and depending on the charge position we either get smectic or nematic behavior (see Figure 1b). A systematic study of the influence of the charge position on the nematic/smectic behavior and phase diagrams of different charge positions will be presented.

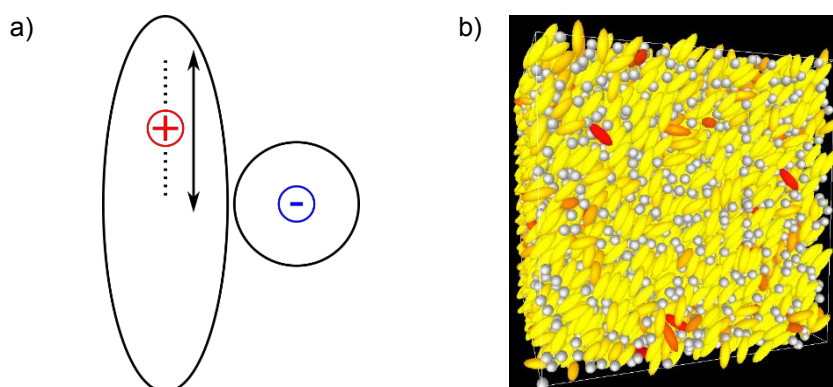


Figure 1: a) Cationic Gay-Berne (GB) particle and anionic Lennard-Jones (LJ) particle. The charge position on the GB particle is varied between simulations. b) Simulation snapshot of a nematic phase. In this case the charge is positioned in the middle of the GB particle.

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Approaching the holy grail of liquid crystal science - biaxial nematic phases from roof-shaped mesogens

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The biaxial nematic phase – a liquid with orientational long-range order along three different directors – has been predicted already in 1970.[1] Various periods of intense research in the area of low weight thermotropic LC's did not deliver any general accepted biaxial nematic material.[2] In our basic effort to find mesogens with a maximum molecular biaxiality in the family of shape-persistent scaffolds, we recently discovered anthraquinone derivatives **1**, which are not only board-shaped, but the steric congestion at the core results in an roof-shaped molecule.[3] In this series of mesogens a lead structure **1** ($R^{1,2} = \text{OC}_5\text{H}_{11}$, $R^3 = \text{OC}_6\text{H}_{12}\text{COOEt}$) with a broad nematic range was identified, which is already close to the maximum molecular biaxiality according to Straley,[4] when the interdigitation of aliphatic chains is taken into account. First results indeed point to the existence of biaxiality in the nematic phase. In the present contribution the molecular structure is optimised starting from the lead structure **1** by varying the nature of lateral and terminal flexible chains (see Figure). In particular the structure and nature (aliphatic, fluorinated chains) of R^2 and R^3 is changed while R^1 equals C_3H_7 . We intend to find an enantiotropic nematic phase below 100°C with improved biaxiality and alignment. The thermotropic properties are studied by POM (Orthoscopy and Conoscopy), DSC and X-ray scattering of magnetic field aligned samples.

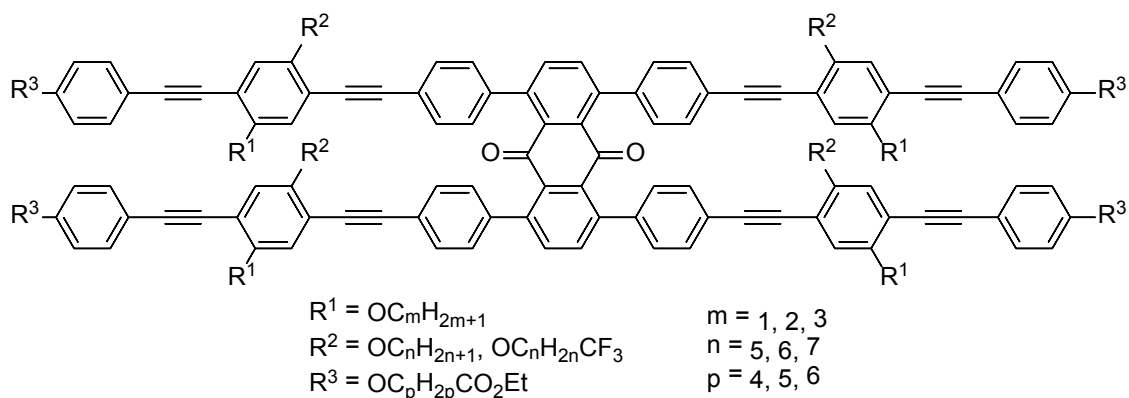


Figure 1. General structure of roof-shaped nematogens.

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- [3] M. Lehmann, S. Maisch, N. Scheuring, J. Carvalho, C. Cruz, P. J. Sebastião, R. Y. Dong, *Soft Matter*, **15**, 8496-8511, (2019).
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Synthesis and Characterisation of a PBI Substituted Oligothiophen-Star Mesogene

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Hexasubstituted benzenes with alternating building blocks around the core, one being a conjugated arm with peripheral long alkyl chains and the other a phenyl group, have been shown recently to be endo receptors for guests and pseudo guests.[1] With this design concept, columnar phases of different structure and stability can be assembled. [2]

In the present contribution, we design a complex alternating crowded mesogen with oligothiophene conjugated arms (Figure 1). In the cavities PBI Acceptors are attached via long spacers. The synthesis of this new sophisticated donor acceptor-mesogen is described and the structure-property relationship is studied by means of POM, DSC, XRS, UV-Vis- and fluorescence spectroscopy.

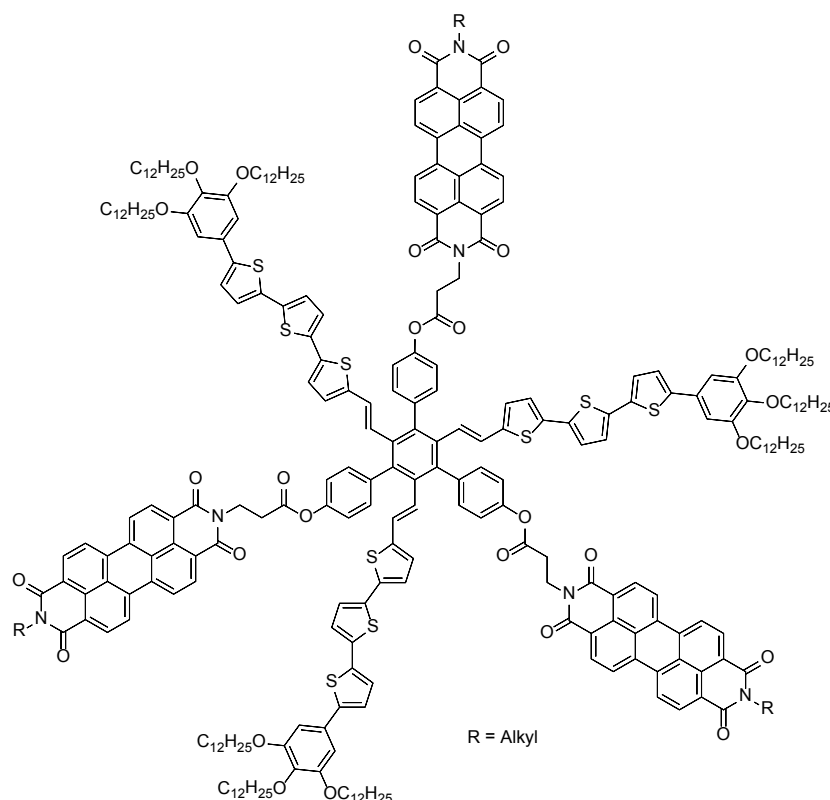


Figure 1: Structure of the target molecule.

References:

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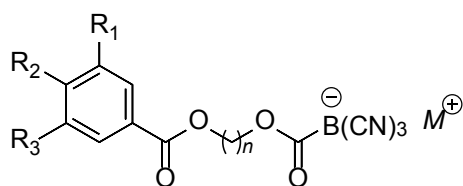
Systematic Study of Ionic Liquid-Crystalline Tricyanoborates Forming Smectic Mesophases

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Ionic liquid crystals (ILCs) are almost as long known as liquid crystals themselves.^[1] Owing to the ionic building blocks and the strong cohesive energy density difference with aliphatics, they form almost exclusively positional ordered lamellar, columnar or cubic mesophases. Well-aligned ionic liquid crystals are interesting materials for new LC electrolytes with high ion conductivity. Frequently, stable organic cations are combined with mesogenic units, while the anions are the stable small counter ions like halogenid ions, BF_4^- or PF_6^- .^[2-4]

Boron anions directly linked to mesogenic units are rarely investigated.^[3, 5] Therefore, we combine here tricyanocarboxy borates^[6] by Steglich esterification with non-polar peripheral groups via a spacer of different length (Figure 1). The liquid crystal properties are investigated as a function of number of peripheral dodecyloxy chains, the spacer length and the nature of the cationic counter ion. The structure property relationship is discussed on the basis of POM, DSC and XRS studies.



$n = 2-4$; $M = \text{N}^n\text{Bu}_4$, [K[18]crown-6]

1-Nⁿ: $\text{R}_1 = \text{R}_3 = \text{H}$, $\text{R}_2 = \text{OC}_{12}\text{H}_{25}$

2-Nⁿ: $\text{R}_1 = \text{R}_2 = \text{OC}_{12}\text{H}_{25}$, $\text{R}_3 = \text{H}$

3-Nⁿ: $\text{R}_1 = \text{R}_2 = \text{R}_3 = \text{OC}_{12}\text{H}_{25}$

N: TBA ($M = \text{N}^n\text{Bu}_4$) or **K** ($M = [\text{K}[18]\text{crown-6}]$)

Figure 1: Overview of the synthesized compounds.

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Umbrella-shaped LC star subphthalocyanines – E-field orientable polar mesophases

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Polar and ferroelectric LC phases are highly interesting owing to their stimuli responsive properties in the presence of an electric field. Besides chiral calamitics and discotics also non-conventional achiral bent-shaped and umbrella-shaped molecules may form such phases (Fig. 1A).[1] Subphthalocyanine-based thermotropic LCs are known to form pyroelectric mesophases after alignment when cooling down from the isotropic phase with an applied electric field.[2,3] Such polar phases can exhibit a bulk photovoltaic effect without a p-n junction as a result of the high phase polarity.[3] Here we present new star mesogens **SP1-3** based on subphthalocyanine cores. They possess a broader absorption in the visible spectral range than previous LC subphthalocyanines and the low clearing enantiotropic columnar mesophases can be homeotropically oriented in the presence of an electric field. The free space between the arms is filled by the formation of parallel oriented dimers. In analogy to the previous discovered CLICK-procedure,[4] the mixture of mesogens without fullerenes **SP1** and sterically overcrowded derivatives with three fullerenes **SPF1** should result in extremely polar bulk-hetero junction materials, which might become of interest for the application in LC photovoltaics. The mesomorphic and polar properties are studied by POM, DSC, XRS and SHG.

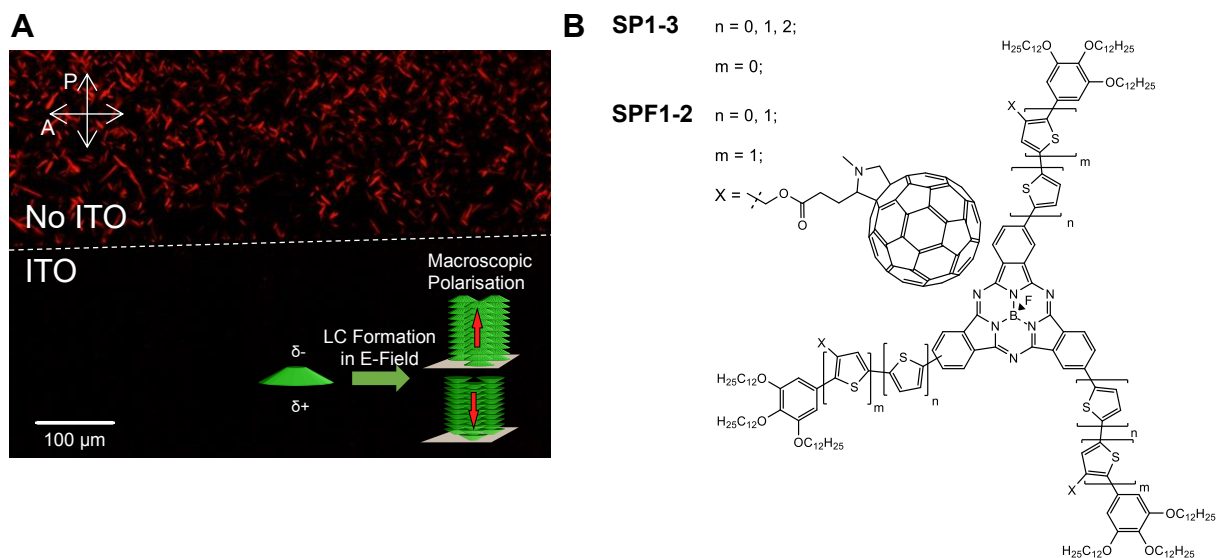


Figure 1: A) POM-texture showing polar columnar mesophases of umbrella-shaped compound **SP2**. B) Structures of target molecules **SP1-3** and **SPF1-2**.

- [1] T. Kato, *Science*, **295**, 2414-2418, (2002).
- [2] T. Torres, *et al.*, *Journal of Materials Chemistry C*, **3**, 985-989, (2015).
- [3] F. Araoka, *et al.*, *Journal of American Chemical Society*, **142**, 3326-3330, (2020).
- [4] M. Lehmann, *et al.*, *Liquid Crystals*, **46**, 1985-1994, (2019).

Orientationally ordered structures in a single flexible-semiflexible multi-block copolymer chain: flat histogram Monte Carlo simulation

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We study conformational properties of a single multi-block copolymer chain consisting of flexible (F) and semi-flexible (S) blocks with equal composition of F- and S-units and with different affinity to a solvent. We perform Monte Carlo (MC) simulations based on the stochastic approximation Monte Carlo (SAMC) algorithm [1,2] which is one of the most recent realizations of the flat-histogram-type MC algorithms [3]. Such algorithms are based on the idea of equally frequent sampling of all energy states of the system and accumulating the density of states function. They sample the configuration space of molecular systems much more uniformly than standard importance sampling MC methods (like, e.g., Boltzmann sampling in canonical MC simulations), and are a powerful tool for obtaining accurate information on phase transitions in molecular systems [3]. In our realization of SAMC algorithm [4-7], we use the two-dimensional density of states function, which depends on the energy of intramolecular stiffness and on the energy of non-valence interactions.

We present data on different non-trivial globular morphologies, including several structures with high orientational ordering of bonds, which we have obtained in our model for different values of the chain length, the block length and the stiffness parameter. Diagrams of states (pseudo-phase diagrams) in variables temperature vs. stiffness parameter are presented for different values of the block length. We compare our results with those obtained previously for a single SF-copolymer chain in a non-selective solvent [4-6] and discuss the observed differences [7].

We also present our recent results on the aggregation behavior of several flexible-semiflexible multi-block copolymer chains and discuss the possibility of shape-persistent aggregation.

We acknowledge the financial support from RFBR (grant 19-53-12006-NNIO-a) and DFG (project PA 473/18-1). We thank Moscow State University Supercomputer Center for providing the computational resources.

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- [2] F. Liang, C. Liu, R. J. Carroll, *J. Amer. Stat. Ass.*, **102**, 305, (2007).
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- [7] D. Maltseva, S. Zablotskiy, J. Martemyanova, V. Ivanov, T. Shakirov, W. Paul, *Polymers*, **11**, 757 (2019).

Siloxane decorated Star-shaped Phthalocyanines as Low Clearing Functional Liquid Crystals

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Star-shaped, shape-persistent liquid crystals (LCs) possess conjugated arms which are symmetrically attached to a core and thus, provide intrinsic free space. When sterically crowded star-mesogens with fullerenes attached through spacers are added, the mixture is reported to produce highly organized materials via a new “CLICK”-procedure. Such structures are attractive for the study as potential photovoltaic devices.[1] One major challenge with this material is the alignment, which was not achieved owing to the high clearing temperature and its decomposition.

The present target molecule **ZN-PC-Si** has a phthalocyanine core and oligo(phenyleneethynylene) arms. The sterically overcrowded derivative **Zn-PC-Si-F** possesses four fullerenes attached via spacers. In order to obtain low clearing temperature, swallow-tailed flexible siloxane chains are incorporated at the periphery of the molecule.[3] Decrease in the clearing temperature well below 200°C is expected, which will enable the homeotropic alignment of the columnar liquid crystals [2]. The structure-property relationship will be investigated by means of polarized optical microscopy, differential scanning calorimetry, comprehensive X-ray scattering and modeling.

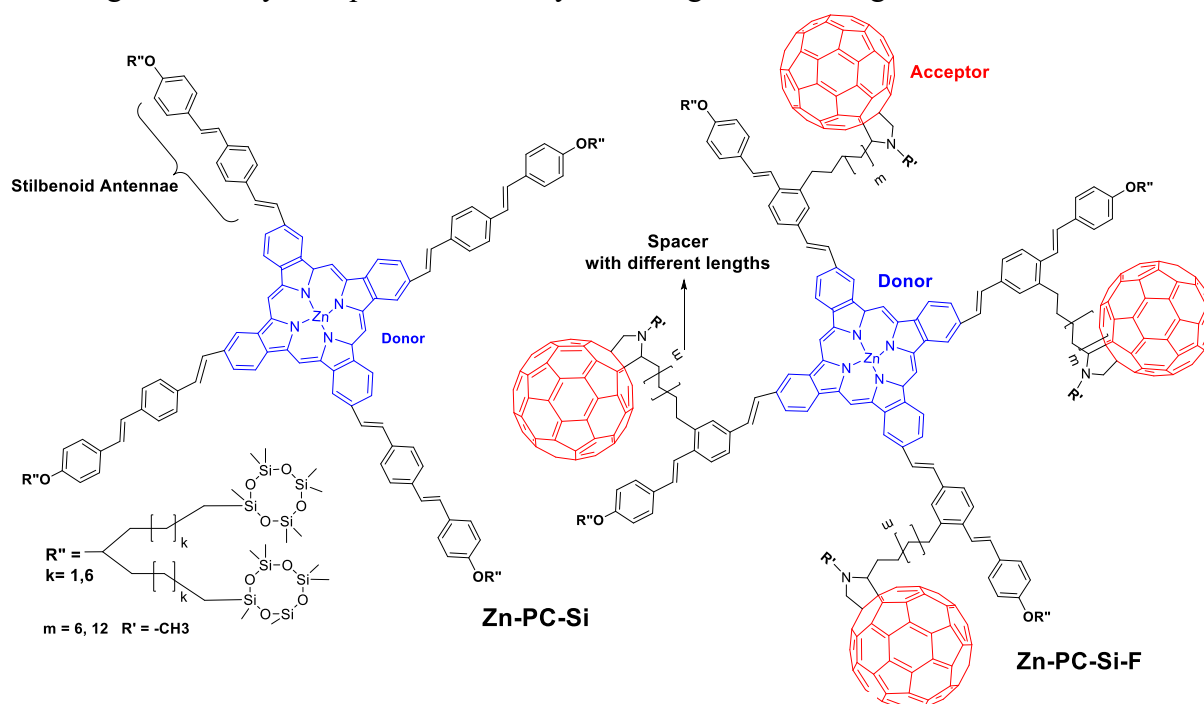


Fig.1 : Zn-PC-Si and Zn-PC-Si-F molecules

[1] M. Lehmann, *Liq Cryst.* **46**,1985-1994, (2019).

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Photosensitive Liquid Crystals Derived from 4-Halogenoresorcinols

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We present novel series of photosensitive hockey-stick liquid crystals. The design of novel materials was inspired by previously prepared compounds (Fig. 1 a)), which we used as intermediates for preparation of bent-core liquid crystals. Surprisingly, these intermediates showed wide temperature range mesophases.¹

In this study, we have varied the molecular structure of the presented materials in several ways to establish the structure-properties relationship (Fig 1. b)). We have introduced lateral fluorine atoms near the azo group to modulate the photosensitive properties.² In addition, derivatives of different length have been used for alkylation or acylation of the free hydroxy group opposite to the photosensitive side arm. We have also varied the halogen atom on the resorcinol core. Subsequently, the mesomorphic behaviour of the prepared materials has been determined by observation of characteristic textures in optical polarizing microscope and measurement of phase transition temperatures by differential scanning calorimetry.

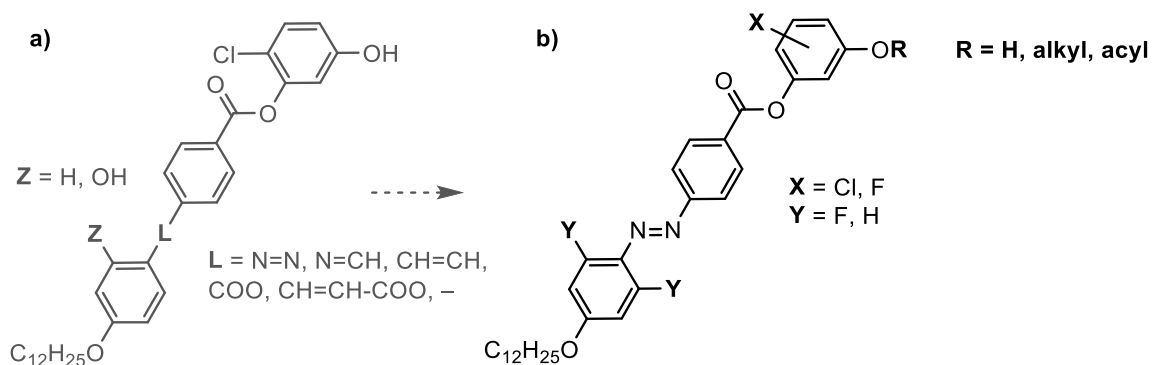


Fig. 1 a) Previously prepared materials b) Final structure of the novel materials

This work was supported by Czech Science Foundation (reg. No. 19-03564S).

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Electric properties of ferro- and antiferroelectric phases in racemic mixture

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A new compound exhibiting antiferroelectric and ferroelectric phases has been synthesized in both chiral versions. The racemate was prepared. Electric responses of a pure enantiomer, as well as a racemic mixture, were studied. Racemization reduces the number of modes observed in electric response as well as their strengths. The strong Goldstone mode, existing in the ferroelectric phase in enantiomer, does not completely disappear in the racemate. Its strength is significantly reduced. The P_H mode, existing in the antiferroelectric phase in the enantiomer, disappears completely in the racemate. Two next modes presented in SmC_A^* : P_L and S still exist in the electric response of racemate. Their strengths change a little. The results show that reduced Goldstone mode in the racemic SmC phase is the continuation of P_L mode observed in the racemic SmC_A phase. It means that both modes P_L in SmC_A^* and Goldstone mode in SmC^* are of similar origin. When we observe both modes in SmC^* and SmC_A^* phases measured in pure enantiomer, it is difficult to compare them. In racemate the strengths of both modes are similar and hence they are easy to compare. Still, the mystery is why P_H mode completely disappears in the racemate. But it seems that it is a rule – we have found this effect in several racemates.

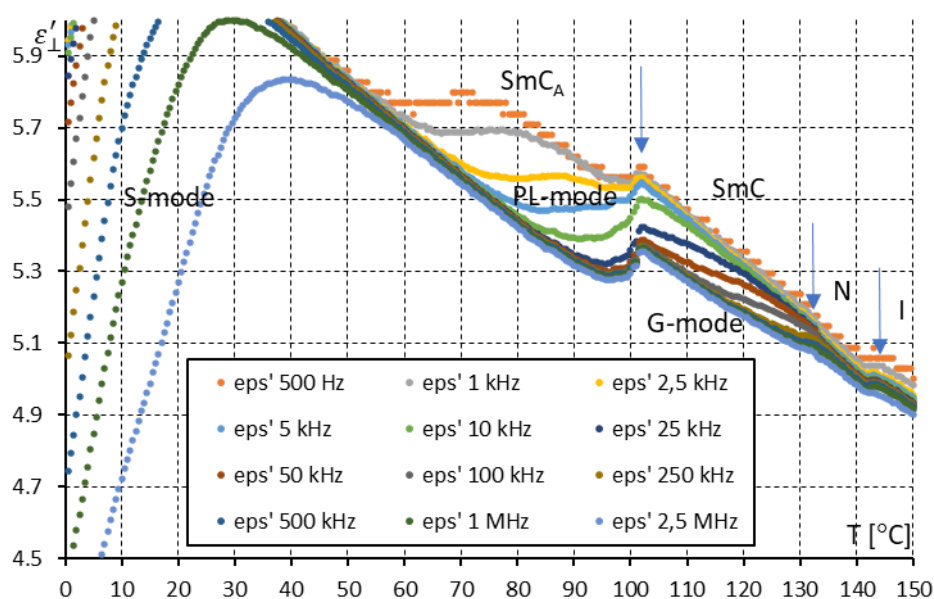


Figure. The real part of permittivity ϵ'_1 , measured versus temperature T for racemate in a planarly oriented cell for several frequencies. Four phases are detectable SmC_A , SmC , N , and I .

Synthesis of Star-Shaped Alkoxy- and Chloro-Triphenylbenzenes: Suzuki Coupling in the Presence of Halogenated Precursors^[1]

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The synthesis of new triphenylbenzenes **2** which represent an extension of already known derivatives **1**, including a further substitution pattern and partial substitution of alkoxy chains with chlorine, is reported (Fig. 1, left). The compounds **2** were obtained by Suzuki-Miyaura cross coupling via two routes, well-established coupling of aryl boronic species **3** (*N*-methyliminodiacetic acid (MIDA) boronates) and 1,3,5-tribromo-benzene **5** (route A) or alternatively, aryl bromides **4** and 1,3,5-trisboronic benzene species **6** (pinacole boronate) (route B) (Fig. 1, top right). Their liquid crystalline behaviour was investigated by DSC, POM and SAXS/WAXS (Fig. 1, bottom right).

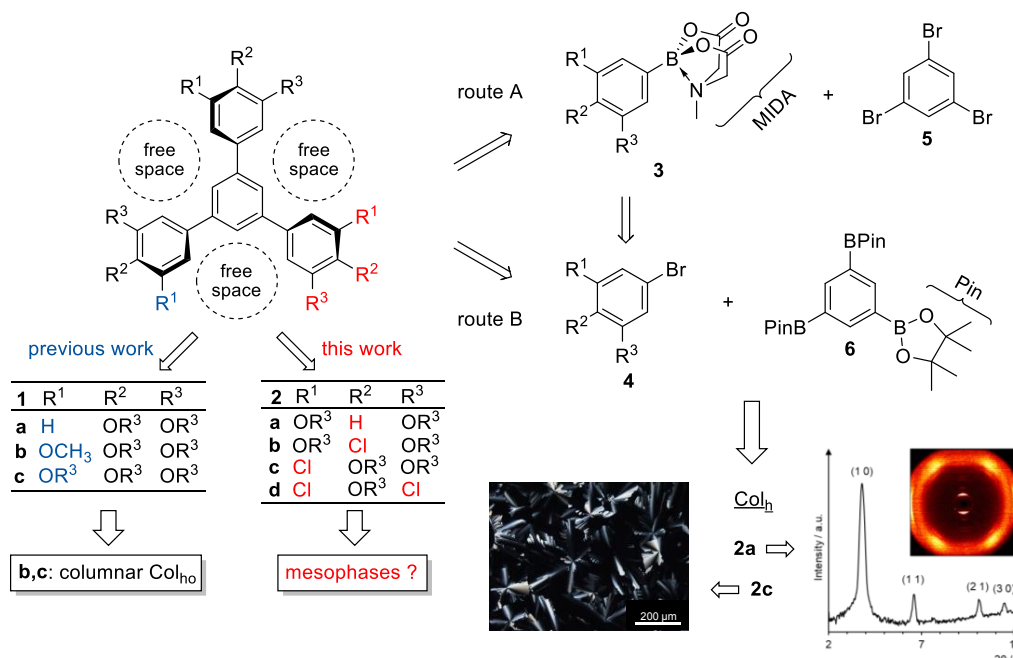


Fig. 1. Comparison of known triphenylbenzenes **1** and new derivatives **2** (left). Retrosynthesis of **2** via two different routes, switching functionalities (top right), and observed Col_h phases for derivatives **2a** and **2c** (bottom right). Figure taken and edited from ref. [1].

The presence of additional halogens can lead to further couplings on route A and thus to undesired by-products. By switching the synthesis to Route B, couplings take only place on the core and further conversion is prevented, leading to a simpler purification and an increase in the overall yield. While for triphenylbenzenes **2a** and **2c** Col_h phases were observed, the position (**2b**) or amount (**2d**) of chlorine in the molecule did not seem to be sufficient to form stable mesophases. Based on SAXS results, a helical packing model was proposed for **2a** and **2c** (structural similarity). Additionally, inhibition of crystallisation was observed when chlorine was involved in the molecular structure, which is mainly attributed to the size and polarity of the atom.

[1] M. A. Grunwald, T. Wöhrle, R. Forschner, A. Baro, S. Laschat, *manuscript submitted*.

Marangoni flow in freely suspended smectic films

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Next to their application in display technology, liquid crystals (LC) are enormously attractive in the field of fundamental physics. Smectic mesophases can form free-standing films with an aspect ratio larger than 10^6 (width to film thickness). These unique fluid structures have been successfully exploited in the past for manifold hydrodynamic experiments, but almost exclusively under isothermal conditions.

In our study, we focus on thermally driven effects in such films. We present the results of microgravity experiments during two suborbital rocket flights, and show that thermal gradients within the film plane can cause huge thermocapillary (Marangoni) effects. The experimental setup to induce temperature gradients in the film plane is sketched in figure 1. In contrast to former experimental studies by Godfrey and van Winkle [1] we avoid a meniscus connecting the two thermoposts.

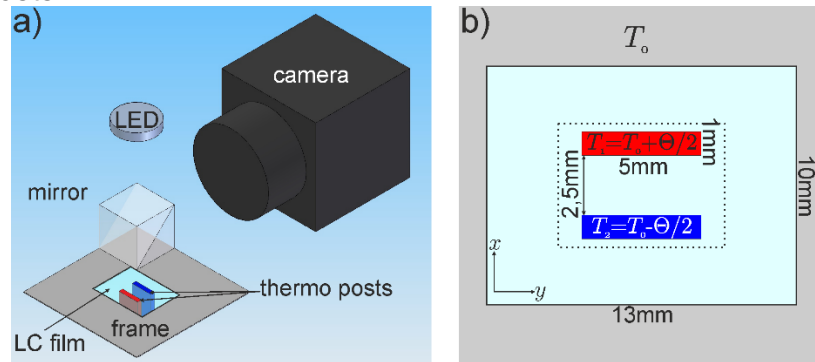


Figure 2: left: schematic image of the experimental setup; the film is observed in reflection via a semi transparent mirror. right: top view of the experimental situation; the film environment is set to a constant ambient temperature T_0 . Between the thermocontacts we could apply temperature differences up to 25 K.

We demonstrate that the temperature dependent surface tension $\sigma(T)$ is the elicitor of flow within the film plane from the hot to the cold film edge for materials with a normal temperature coefficient of the surface tension ($d\sigma/dT < 0$). Finally we provide a hydrodynamic model that describes our experimental findings quantitatively [2]. Surprisingly, the temperature difference is the relevant control parameter. This is in contrast to Benard-Marangoni or Rayleigh-Benard convection, where the temperature gradient plays the essential role.

The study was supported by the German Aerospace Center (DLR) within projects 50WM1430 and 50WM1744.

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Study of a novel chiral glass-forming liquid crystal

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There is a wealth of materials for which a glassy state appears as a result of cooling, and capable of undergoing subsequent cold crystallization during heating. Some liquid crystals can be found among such materials [1,2]. Glass-forming substances are continually the subject of scientific research due to their properties and potential applications. Today a novel chiral mesogen, capable of assuming smectic (SmC_A^*) phase with antiferroelectric properties, will be presented, Fig. 1. The compound under study is a fluorinated liquid crystal, which gained attention among liquid-crystals researches as a promising compound for the use in new-generation liquid-crystal displays. Its phase polymorphism, as well as relaxation and vibrational dynamics will be discussed. We are aiming at the understanding of many factors influencing its structural and dynamic properties, as well as its ability to form glass from the SmC_A^* phase. Research was being conducted by complementary methods, e.g. differential scanning calorimetry (DSC), polarized optical microscopy (POM), Fourier-transform infrared spectroscopy (FTIR) and broadband dielectric spectroscopy (BDS) [3,4]. The latter was carried out under ambient and elevated pressure, by means of a dedicated attachment. In this way, the ability of the tested compound to crystallize from the SmC_A^* phase under changing thermodynamic conditions could be better understood. There are few works dealing with high-pressure crystallization at different temperatures for organic glassformers.

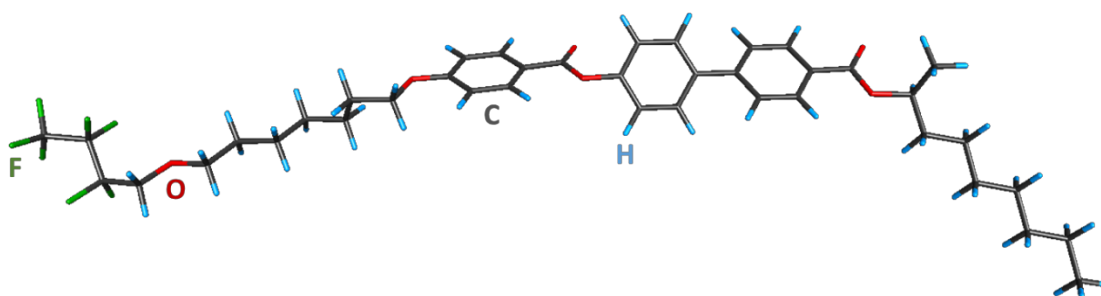


Figure 1. General structure of (S)-4-[7-(2,2,3,3,4,4,4-heptafluorobutoxy) 4'-(1-methyloctyloxycarbonyl) biphenyl-4-yl heptyloxy] benzoate (abbreviated as 3F7HPhH7), optimized with DFT method.

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Relationship of cold crystallization kinetics and molecular dynamics in 3F5HPhH compound

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The chiral fluorinated 3F5HPhH compound [1] undergoes the glass transition from the antiferroelectric smectic C_A^* phase for cooling rates ≥ 5 K/min, followed by the cold crystallization on heating [2] (Figure 1). The non-isothermal cold crystallization ($SmC_A^* \rightarrow Cr2$) and subsequent secondary crystallization ($Cr2 \rightarrow Cr1$) are investigated by differential scanning calorimetry for 1-20 K/min heating rates. Different values of the energy barrier for cold crystallization are found for slow (1-5 K/min) and fast (8-20 K/min) heating. Additionally, molecular dynamics in the smectic and crystal phases of 3F5HPhH is studied by broadband dielectric spectroscopy, with special attention to the α -process in the smectic C_A^* phase (attributed to molecular rotations related to the smallest moment of inertia) and the relaxation process in crystal phases (attributed to intra-molecular rotations based on DFT calculations). The coupling between the relaxation time of the α -process and characteristic time of the cold crystallization (in isothermal approximation) is determined according to the method presented by Ediger et al. [3].

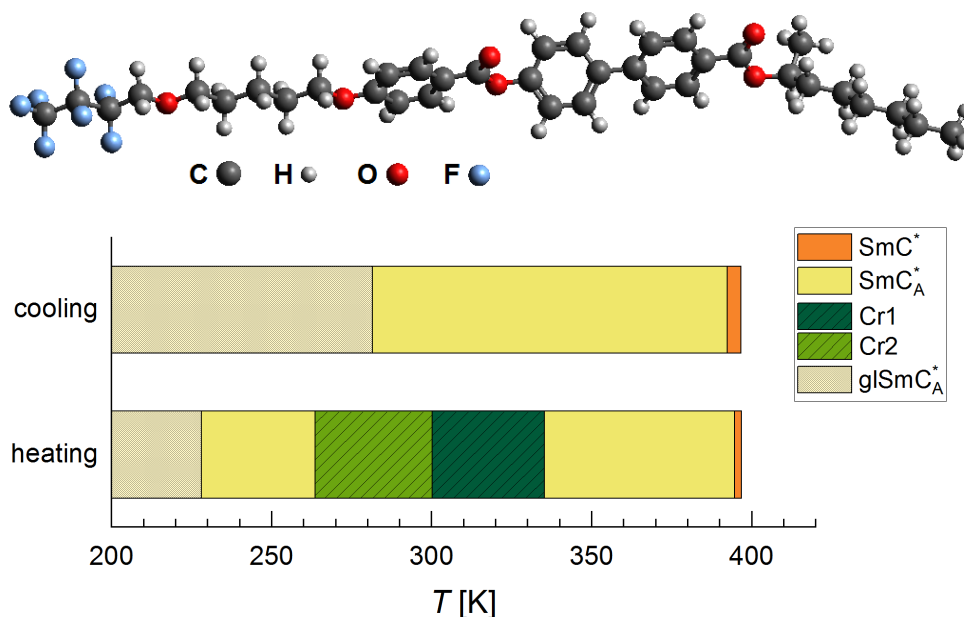


Figure 1. 3F5HPhH molecule optimised with DFT-B3LYP/def2TZVPP calculations and phase sequence of 3F5HPhH for 5 K/min rate.

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Molecular origin of the heterogeneity in the nematic and smectic liquid crystals: elastic constants, gradients of order parameters and visualization of small objects

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The formation of heterogeneous nematic and smectic liquid crystals in the general case of an arbitrary geometry is investigated in the framework of molecular-statistical approach. The importance of theoretical consideration of the distorted smectic and nematic substances is well understood from the appearance of new LC phases [1–2] in the presence of director deformation. We are going to follow the idea that smectic

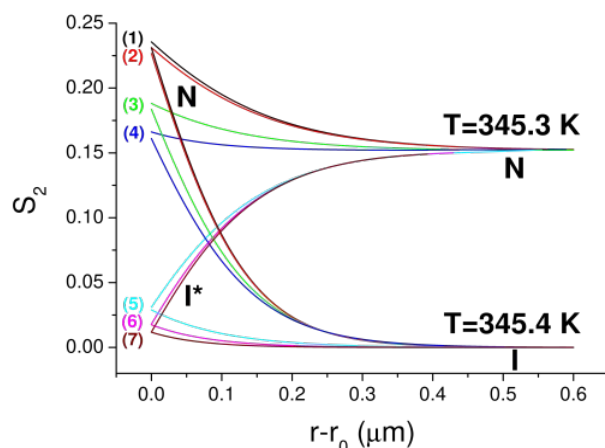


FIG. 1. The dependencies of the prime orientational order parameter on the distance $r - r_0$ from the particle's surface just below (at $T = 345.3\text{K}$) and just above (at $T = 343.4\text{K}$) the nematic-isotropic transition temperature in the bulk of LC at various sizes of the particles: (1) $r_0 = \infty$ [flat surface]; (2) 10; (3) 3; (4) 2.5; (5) 1.9; (6) 1.55; and (7) 1.25 μm .

layering is similar to the microphase separation in polymers [3 – 4]. The orientational and translational orderings at the curved surfaces of small solid objects dispersed in liquid crystal (LC) are considered, and the differential equations for gradients of the order parameters in vicinities of the small objects are presented in the general form. The five elastic constants are obtained within the same approach, from which we were able to predict that a significant space variations of the order parameters can be observed within the 0.5 – 0.8 μm area around any small object, almost independently of its own dimension. Therefore, the liquid crystals can be a simple tool for the optical visualization of nanoobjects.

Acknowledgements. This project was supported by the Russian Foundation for Basic Research (Project No. 19-53-52011 MHTa). The work of E. S. F. was done in the frame of the International Graduate School AGRIPOLY supported by the European Social Fund (ESF) and the Federal State Saxony-Anhalt.

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Mesomorphism and photochemistry of (E)-4-((4-decyloxyphenyl)diazenyl)phenyl alkanoates

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Compounds containing diazenyl group ($R-N=N-R'$) are very fruitful field of research due to combination of mesogenic and light-sensitive properties. It is important to obtain new compounds of this kind especially for optoelectronic applications [1].

In this work a new homologous series of (E)-4-((4-decyloxyphenyl)diazenyl)phenyl alkanoates was synthesized to check the effect of length of the hydrocarbon chain of the alkyl acid on the phase transition temperatures and the type of mesophases occur (Fig.1). Nematic phase was observed for derivatives up to $m = 11$. From propanoate derivative ($m = 2$) occurrence of SmC phase was noted. Except these mesophases also SmA, SmI, SmF and G phase were observed. Number of mesophases can also be modulated by changing the length of the alkyloxy chain [2,3].

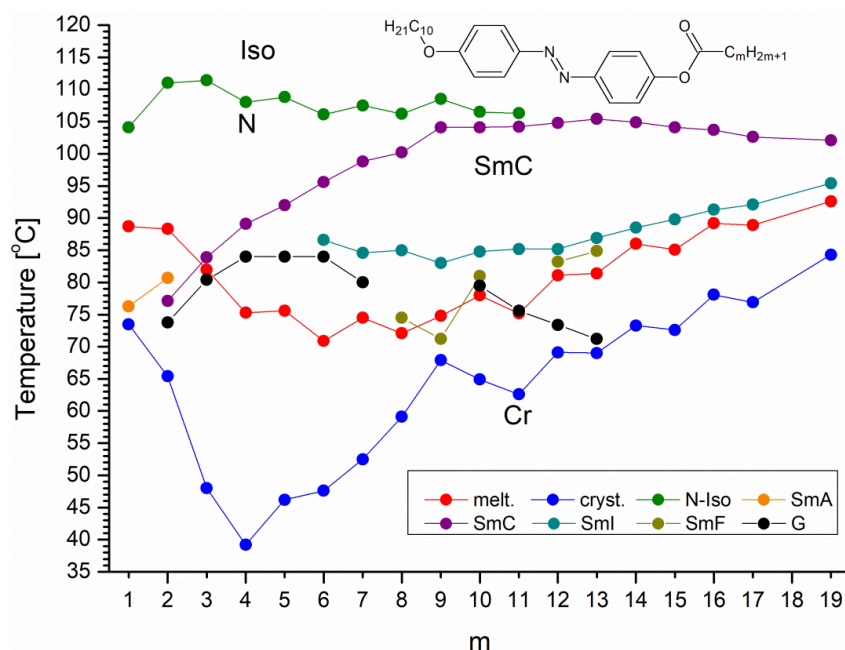


Fig.1. Phase situation of (E)-4-((4-decyloxyphenyl)diazenyl)-phenyl alkanoates based on TOA method (rate of temperature changes 10 K/min).

Temperatures of the N-Iso transition show the odd-even effect. Unusual behaviour of the first two derivatives of the homologue series was noted. Physicochemical properties were obtained using POM, TOA, DSC, XRD, FTIR and BDS methods.

Derivatives of this series absorb UV-Vis light causing trans-cis isomerization processes. Kinetic coefficients are typical for this class of compounds.

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Using Cyanobiphenyl-based Liquid Crystal Droplets to Detect Volatile Gases

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Gas sensing is an emerging research field relevant to almost every aspect of our modern society from households to health facilities, industrial units, even military environments. Sensor features such as high sensitivity, selectivity, fast response and low energy consumption are essential. Liquid crystals (LCs) are excellent candidates for the design of sensing platforms, considering that their electro-optical properties change upon interaction with analytes. We have recently developed a formulation for novel hybrid LC gels, emerging from the cooperative assembly of LC-ionic liquid (IL) droplets within a biopolymeric matrix [1,2]. Exposing the gels to volatile organic compounds (VOCs) results in either a phase transition or a reduction of the order parameter as observed by polarised optical microscopy. In this work we investigated the variation of the LC component in the assembly and molecular organisation of the hybrid gel, while keeping the IL and biopolymeric matrix constant. The LCs studied include nematic and smectic cyanobiphenyl-based compounds. We characterised the morphology of the LC-IL droplets formed and the LC director configuration within the droplets. We also compared our results with the control compositions, where either the IL or the LC were absent. Secondly, we studied the potential of our gel compositions as sensing elements in a custom-built prototype e-nose, a device designed to mimic biological olfactory systems, exposing them to a sequence of VOCs representative of distinct groups (such as alcohol, ketones, aliphatic, aromatic and halogenated compounds). We demonstrate that the collected optical responses to the presence of analytes enable the distinction and automatic classification of VOCs using machine-learning algorithms. This shows an unprecedented example of soft matter in molecular recognition and artificial olfaction, where hybrid gels can provide enough information to accurately classify VOCs with very small structural differences.

Acknowledgements: This work has received funding from the European Research Council through the grant reference SCENT-ERC-2014-STG-639123 (2015-2022). This work was supported by the Applied Molecular Biosciences Unit – UCIBIO (UIDB/04378/2020)

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Surface Modification with Benzophenonesilane Derivatives for Liquid Crystal Test Devices

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Benzophenonesilane (BPS) is a promising agent for surface functionalization in liquid crystal (LC) devices. The two functional groups in BPS molecules, a chlorosilane group and a benzophenone moiety, are separated by an aliphatic spacer. The chlorosilane group facilitates covalent surface attachment, while the benzophenone group is a well-known photoinitiator for radical polymerization reactions. There are different possibilities to use such a surface-grafted photoinitiator (SGPI) in LC devices, e. g. substrate modification for LC test cells [1,2] or surface functionalization of inorganic particles [3] for doping of a LC host. A well-known synthesis route [4] has been found to be suitable [5] to synthesize a variety of BPS homologues with a spacer length of 3 to 12 carbon atoms. The deposited monolayers could be conveniently studied by ellipsometry: Using piranha etched silicon wafers [1] or silicon wafers with a thin native oxide layer of known thickness [5] was found to result in reliable thickness measurements. To compare the coatings on different kinds of substrates, contact angle measurements were used for characterization (Figure 1). The contact angle of the photochemically active monolayers could indeed be varied upon photo exposure [5].

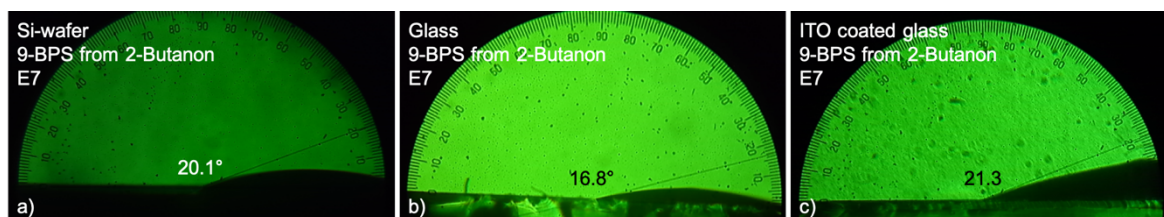


Figure 3: Contact angle of the nematic LC E7 on surfaces modified by spin-casting a solution of 9-BPS in 2-butanone on different substrates a) silicon wafer, b) microscope slide, and c) ITO coated glass.

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Electrically tunable diffraction and anomalous refraction by metasurfaces made of nematic liquid crystal

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Metasurfaces open up new horizons in optics: their unique properties allow for creation of flat devices with diverse functionalities, such as polarization or wavelength selective filters, diffraction gratings, lenses, holograms, and many others. The impressive optical properties are designed by optimizing the periodical arrangement of specific resonant meta-atoms.

We put forward the idea of soft metasurfaces entirely based on liquid crystal (LC), which bring in the advantage of fast electro-optical switching. Spatially-periodic nematic LC modulation is

imposed by periodical surface alignment conditions created by focused-ion-beam patterning of initially planar alignment layer rubbed polymer) that locally changes the anchoring from planar to vertical. Given a micrometer periodic stripe pattern consisting of alternating treated non-treated stripes, the director of adjacent LC follows the anchoring, swinging between the mutually orthogonal directions [1]. The grating-like patterns determine pronounced colouring the metasurfaces, depending on period (Fig.1,a), and produce strong diffraction (Fig.1,b). Multi-parametric optimization of metasurface design [2] allows for achieving more complex diffraction patterns, such as strongly asymmetric diffraction with up to 60% of light directed into a single particular channel (Fig.1,c), effectively resulting in efficient anomalous refraction. The diffraction efficiency is further enhanced and the spectral range broadened with double-sided metasurface design, based on optimized patterns produced on the both substrates of the LC cell and synchronized.

The metasurfaces are electro-optically switched during milliseconds between the diffraction/anomalous refraction and transmission modes by a voltage of just several Volts applied across the LC layer (Fig.1,d) [2, 3].

The research is funded by the Russian Science Foundation (Project 18-12-00361).

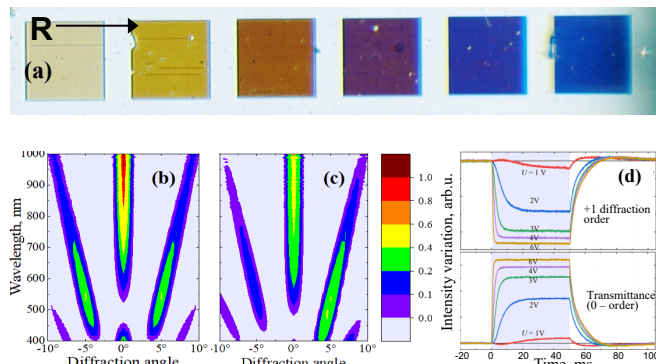


Figure 1. a) Metasurfaces of periods 3 to 8 μm (left to right) in polarized light; **R** indicates the same direction of the polymer layer rubbing, the pattern stripes and the input linear light polarization. Angle–wavelength transmitted intensity maps for the light polarized along **R** normally incident on 6 μm periodic metasurface: b) with periodic stripes of equal width and c) with

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Rheological properties of ferroelectric liquid crystalline materials

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The chiral smectic ferroelectric liquid crystalline (FLC) materials form a very specific by highlighted class of the self-assembling materials with polar ordering which can be used for numerous attractive applications useful for the society needs. Specifically, due to unique properties, the ferroelectric liquid crystals can be effectively used in construction of various optoelectronic devices: light valves, modulators, display devices and small liquid crystalline displays. However, even if the viscoelastic properties are very desirable and important, as they are closely related to the switching time, the available related information for new materials and their mixtures is quite isolated and controversial. The main reason is related to the experimental difficulties, which can occur during the investigations that, in fact, make quite strong contrast with the needs of the research and engineering communities. One of the most significant factors is that the switching time of ferroelectric liquid crystals strongly depends on the mechanical properties, namely on the rotational viscosity of the smectic c-director. Therefore, the precise determination of this adequate parameter is of great importance for successful design of new optoelectronic applications. Most commonly, the measurements of the viscosity coefficient were done using the switching phenomenon but this approach might provide incorrect results. The measurement of viscosity is based on the observation of flow caused by an external force. To ensure correctness of the measurements, the flow should be laminar. It is only the case when the flow stimulating factor (in our case the deformation of the helical structure) is weak. For this reason, the switching method can designate only qualitative but not the quantitative results. In this presentation the electro-optic method has been used for determination of the elastic constant [1] and the rotational viscosity coefficient [2] associated with the smectic c-director in ferroelectric liquid crystalline materials.

The electro-optical method fulfils the conditions of small deformation and laminar flow (see Figure 1). It will be demonstrated that comparing obtained results can give an insight into restructuring processes, which occurs in the studied chiral smectic FLC materials. An additional advantage is the measurement performed exactly in the same cell geometry as the electro-optical panel used in liquid crystal displays. The linear optical tests can be applied as one of the complementary methods for determining the mechanical properties of liquid crystals.

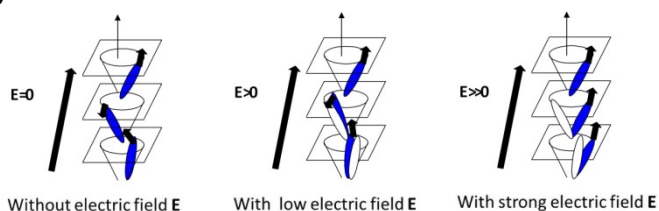


Figure 1. Schematic cartoon representing the behaviour of the ferroelectric smectic phase under applied arrows.

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This work was supported by the National Science Centre (NCN) Poland under Grant 2017/25/B/ST3/00564.

Luminescent, dielectric and contact properties of liquid crystal composites with multilayer quantum dots

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The paper is focused on synthesis of highly luminescent hybrid “core/shell” quantum dots (QDs) with different core sizes and an additional shell. These quantum dots were doped into a nematic liquid crystal (NLC) phase to obtain new composites. According to the dielectric and femtosecond laser spectroscopy data, sizes of the QD cores and built-up additional shells are correlated with luminescence and dielectric characteristics of the NLC and QD composites. With larger QD cores in the NLC ZhK-1282, a decrease in dielectric relaxation frequency of the LC molecules rotating around their short axis is observed, same for the activation energy of this process. A shift to a shorter wavelength of the LC main luminescence peak and the strong luminescence quenching effect can be observed for the composites with the 2 nm QD cores. The adhesion work values have been calculated for all the samples, alignment substances and substrates. Optimized homeotropic aligning layers with the best composite anchoring parameters have been selected both for normal glass and glass with an ITO layer.

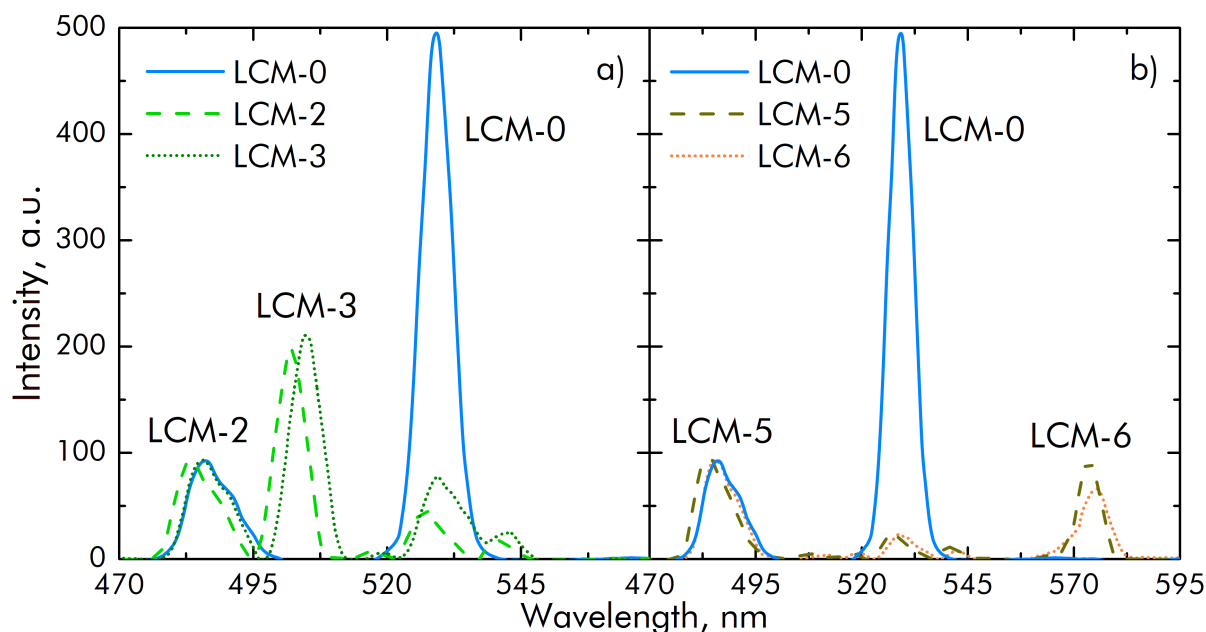


Figure – Luminescence spectra of different LC composites doped with quantum dots with 2 nm (a) and 3 nm (b) cores

Tailored lyotropic liquid crystal templates: Chances and limitations of added co-surfactants and swelling agents

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Mesoporous silica materials, fabricated by direct liquid crystal templating, can be used for a variety of applications, e.g. energy storage, adsorption, drug delivery or heterogeneous catalysis. For successful applications, a precise control of the pore diameter – which is immediately linked to the micelle dimensions of the liquid crystal template phase – is necessary. In literature, it is known, that micelle dimensions can be adjusted by adding co-surfactants [1] or swelling agents [2]. However, these studies lack a clear cut system to establish general rules and identify potential limitations. Thus, we systematically investigated the influence of numerous co-surfactants and swelling agents on the hexagonal lattice parameter and stability of the lyotropic system P123/water by changing stepwise the additive's chain lengths, substituents and concentrations. We explain the partially non-intuitive results by solubility considerations and molecular rearrangements within the micelles.

The transferability to mesoporous silica materials which were templated by the respective lyotropic systems was tested for selected additive systems and concentrations. The materials were characterized by means of X-ray diffraction, N₂-adsorption and TEM measurements, showing that swelling agents and co-surfactants are a powerful tool to fine tune the properties of mesoporous silica materials.

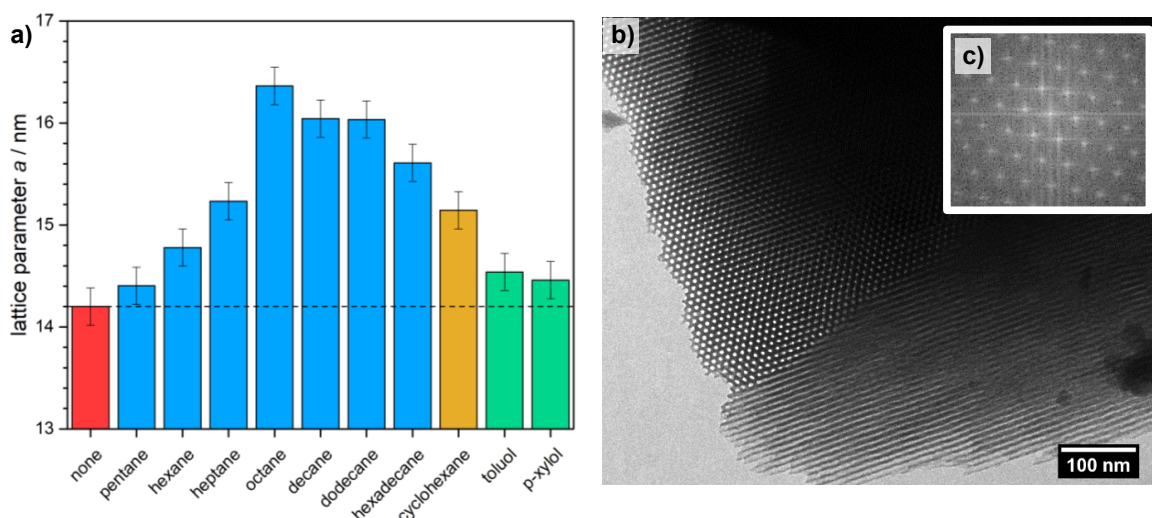


Fig. 1: a) Hexagonal lattice parameter a of the lyotropic system P123/water in dependence of various swelling agents, each with a molar fraction of 1.5 %. b) TEM image of a mesoporous silica material templated from the P123/water/hexane system. c) FFT image of a selected area of b).

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Investigation of Electrospun Liquid Crystal/Polymer Nano-fibers: Effect of Liquid Crystal Type

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A large quantity of research has been done to enhance the physical properties of liquid crystals by combining with polymers. LC/polymer composites can be formed in fiber [1-3]. Recently, electrospinning technique has been frequently preferred as a simple method because of forming micro and nano-sized fibers with a core-sheath structure in which a liquid crystal core is encapsulated with a surrounding polymer cover [4,5]. There are a lot of parameters that affect the physical properties of the electrospun fibers such as type of polymers, solvent, value of the application voltage, distance between the needle and the collector, viscosity of the solution, surface tension, and charge density induced by electrospinning [5].

In this study, it is aimed to observe the change of the fiber structure and some physical properties by using different type of liquid crystals. Polyacrylonitrile which exhibits a very low birefringence and is a hydrophobic [30] was used as polymer. Owing to this property, it is a good candidate as a sheath of the fiber. Some high-birefringent and low molecular weight alkyl based liquid crystals which are member of cyanobiphenyl group were used as a core material. Textures of nano-fibers were obtained by polarized optical microscopy. In order to determine the orientation degree of liquid crystal molecules in the center of fiber, textures were taken at different angles. Also, the morphology and diameter of the nano-fibers were determined using a scanning electron microscopy. Addition to this, thermal properties of electrospun fibers were examined so as to determine the mass change of the nano-fiber over time as the temperature changes. Detailed information will be given in the presentation.

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Large Angle Forward Diffraction by Chiral Liquid Crystal Gratings with Inclined Helical Axis

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Reflective diffraction gratings based on chiral liquid crystals are strong contenders among the other waveguide-coupling components because of their high diffraction efficiency and unique polarization selectivity. In literature, it has been shown that in such devices, the liquid crystal planes with constant director orientation are inclined with respect to the substrate plane. Two director configurations have been reported without experimental proof: one with the director parallel to the substrate[1] and one with the director parallel to the tilted planes of constant director.[2] Previously we reported that the director in the bulk of such a structure is not parallel to the surface and the polar angle of the molecules is not constant.[3] In this work, we provide analytical formulae for azimuthal and polar angles of such a structure.[4] To support our findings we implemented these formulae in a simulation program and compared the results with measurements for a grating with a large inclination angle. In this presentation we present forward diffraction with a lateral shift in diffractive gratings with chiral liquid crystal as illustrated in Fig. 1. We also provide an explanation based on the optical properties of different layers for different polarizations of light.

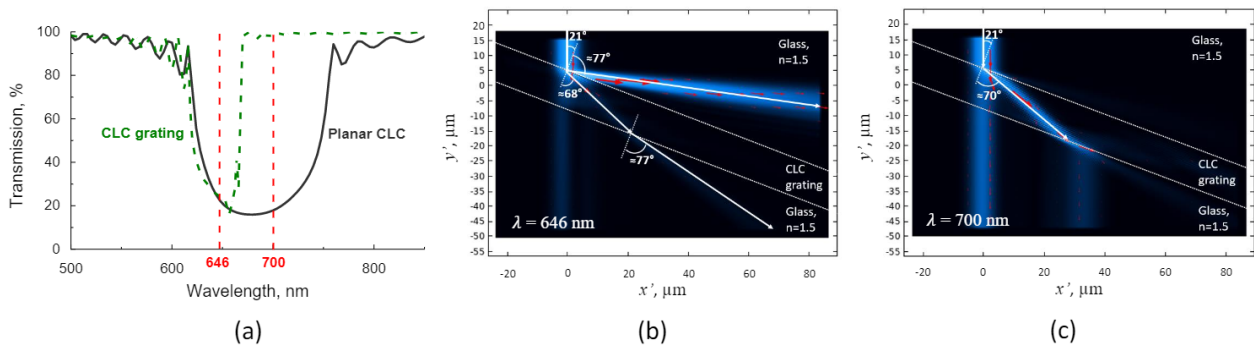


Figure 1. (a) Comparison between transmission spectra for linearly polarized light (-45°) with angle of incidence $\theta_{in} = 21^\circ$ for a CLC grating with a 24° inclined helix (green) and for a planar CLC with angle of incidence 45° (black). Simulated field intensity distribution for a linearly polarized (-45°) Gaussian beam with angle of incidence 21° on an CLC grating with a 24° inclined helix, for wavelengths (b) $\lambda = 646$ nm (mostly reflection) and (c) $\lambda = 700$ nm (mostly transmission).[4]

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Structure of the liquid crystal C8BTBT with high-charge-carrier mobility confined in hydrophilic and hydrophobic anodic aluminium oxide nanochannels

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We investigate the temperature-dependent self-assembly of the liquid crystal C8BTBT within anodic aluminium oxide (AAO) nanochannels as a function of pore width and channel wall chemistry. Results of concerted synchrotron X-ray diffraction experiments and measurements employing a high-resolution optical polarimetry technique are presented. We find a pore-diameter-dependent orientational transition from a radial to an axial orientation of the elongated liquid crystal molecules within hydrophilic AAO nanopores. In ODPA surface-treated, i.e. hydrophobic AAO nanochannels this trend of the orientational order is found to be partially reversed.

Due to the comparatively large beam size of the above experimental techniques, the liquid crystalline structure is probed within a large amount of nanopores at the same time, such that one obtains a respectively averaged structural information. We therefore present preliminary results of an X-ray diffraction experiment with a nanobeam, enabling us to investigate the structure of liquid crystals within individual nanochannels.

Nematic Liquid Crystals for Light Tracducers with High-Transmission of Light and Very Low Reflection at VISible, Near, Short and Medium InfraRed Regions

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Two nematic liquid crystal mixtures IRN1 and IRN2 developed in MUT are discussed. The IRN1 with phase sequence: Cr/−10.0°C/N/+52.1°C/Iso is new high birefringence liquid crystal mixture [1] for special laser rangefinders dedicated to 3D [2] or 5D [3] laser metrology, dense plasma diagnostics [4] and space mission applications [5] working at VIS ($\lambda=0.63\mu\text{m}$) and NIR ($\lambda=1.06\mu\text{m}$) bands. The second mixture IRN2 (Cr/−1.0°C/N/60.9°C/Iso) is prepared for breathalyser application [7] where Liquid Crystal Shutter (3.4LCS) working at the edge of MWIR ($\lambda=3.43\mu\text{m}$) range is applied.

1. IRN1 and IRN2 liquid crystal mixtures

To obtain IRN2 with low absorption at the edge of MWIR window ($\lambda \in [3.0\mu\text{m}, 4.2\mu\text{m}]$) one replaces hydrogen atoms in molecules of IRN1 with the heavier ones, preferably with deuterium or/and fluorine. Such an engineering of mesogens eliminates the high absorption bands at $\lambda \sim 3.4\mu\text{m}$. To obtain high $T > 97.5\%$ and very low $R < 0.5\%$ in refractive index Matched Liquid Crystal Cells (MLCC), all other light losses L in MLCC must be lower than 1.8% ($T+R+L=100\%$). Since A_{LC} (for $\lambda=0.6328\mu\text{m}$) of $15\mu\text{m}$ thick IRN1 layers and A_{QP} of two Quartz Plates (QP) are practically non-measurable ($A=A_{LC}+A_{QP} \sim 0.1\%$) and moreover, Light Diffusion (LD) at boundary surfaces of QP can be practically removed ($LD \sim 0.1\%$) by polishing processes, Diffused Reflection (DR) of $15\mu\text{m}$ layer of IRN1 for MLCC should be not higher than 1.6% ($T+R+A+LD+DR=100\%$). In this situation, DR factor, should be smaller than 1.6% for $15\mu\text{m}$ layer of IRN1 for MLCC. To satisfy the requirement for $DR < 1.7\%$ at $15\mu\text{m}$ of IRN1 the components of IRN1 were further selected, from a two different classes of nematogens with similar birefringence to reduce the possibility of strong heteromolecular interactions; thus are the formations of solid crystal or smectic-like agglomerates. Ordinary n_o and extraordinary n_e refractive indices of IRN1 and IRN2 in VIS, NIR, SWIR and at an edge of MWIR (from $3.0\mu\text{m}$ to $4.2\mu\text{m}$) regions (See Figure 1) were measured by interference method using “special IR cells” with dielectric mirrors [7].

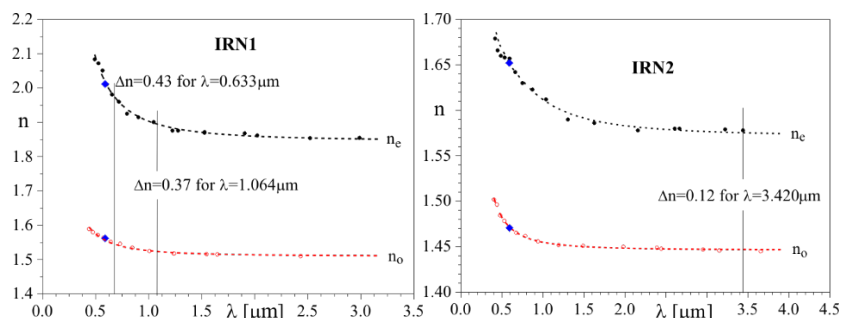


Figure 1: Dispersion of $n_e(\lambda)$ and $n_o(\lambda)$ for IRN1 and IRN2 mixtures at the room temperature.

2. Refractive index MLCC with IRN1 and IRN2

To increase T to the level above 97.5% (see Figure 3), one needs to minimise as much as possible, or even remove, some sources of light losses which appear in

a simple **Twisted Nematic (TN)** and **Electrically Controlled Birefringence (ECB)** cells [1-6]. To lower R of MLCCs at all filled cell interfaces to below 0.7%, MLCCs were designed as a stack of functional, optically matched layers (See Figure 2).

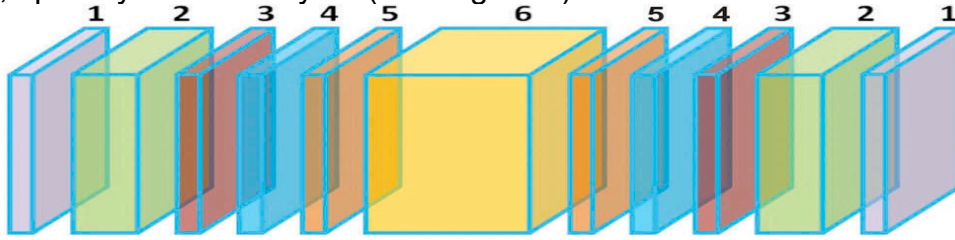


Figure 2: MLCC was constructed as: 1-AR are bilayer, dielectric anti-reflex coatings; 2-QP; 3-ITO are transparent Indium Tin Oxide layers; 4-BL are dielectric SiO_2 blocking layers; 5-AL are polyimide homogeneous alignment layers; 6-IRN1 or IRN2 are LC mixtures.

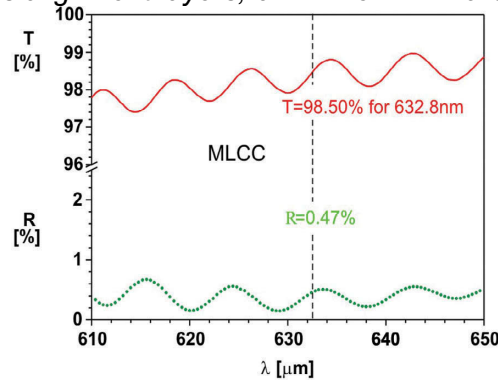


Figure 3: T and R of polarized light versus λ for TN MLCC ($d=13.7\mu\text{m}$) filled with IRN1 ($\Delta n=0.43$ at $\lambda=0.6328\mu\text{m}$ at 20°C). MLCC (when $U=0$) was placed between crossed polarizers.

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Inversion of helical twist sense in three component system showing SmC^*_A phase

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The phenomenon of the twist sense inversion of helical structure within one liquid crystalline phase was found in many compounds and phases [1-2].

Recently the summary of the influence of the chemical structure on the helical pitch changes upon temperature in SmC^*_A phase of many homologous series was presented [3]. Mixing compounds of opposite handedness let obtain the inversion of the helical structure upon concentration [4].

The aim of the presentation is to show that it is possible to obtain the three component system with the inversion of helical structure in SmC^*_A phase. Choosing the right composition it is possible to obtain the inversion of handedness at set temperature in the whole concentration range. Mixtures with high helical pitch are convenient for better alignment of molecules in the devices.

The obtained results prove that the inversion phenomenon is a common behavior and that the value of the inversion temperature can be easily tuned according to the requirements.

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Influence of the ferroelectric BaTiO₃ nanoparticles on some properties of the antiferroelectric binary mixture

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The synthesis routes of organic compounds (like liquid crystals) are complex and expensive. In contrary to synthesis methods, the admixture process synthesized materials is relatively simple and has a lot of potential. The doping can be at the stage of the crystal, liquid crystalline or liquid phase, while the dispersed object can be in a form of a solid, solution or homogeneous mixture and has different concentrations and grains size, etc. The admixture of small particles (nanoparticles) has a little effect on the behavior of the liquid crystal director. On the other hand, nanoparticles (e.g. BaTiO₃, LiNbO₃) are big enough to maintain their ferroelectric properties and share these intrinsic properties with LC matrix. Additionally, the low concentration of nanoparticles prevent agglomeration of nano-objects and the formation of defects. If the nanoparticles concentration is large enough the rigid suspensions can be obtained [1–3]. In this work, we present influence of BaTiO₃ nanoparticles on the physical properties of the antiferroelectric SmC*_A phase. The doping of the antiferroelectric liquid crystal matrix with ferroelectric nanoparticles causes a strong interaction between dipoles of both materials, which leads to change the electrical, optical, dielectric and structural parameters, as it is presented as an example in Fig. 1.

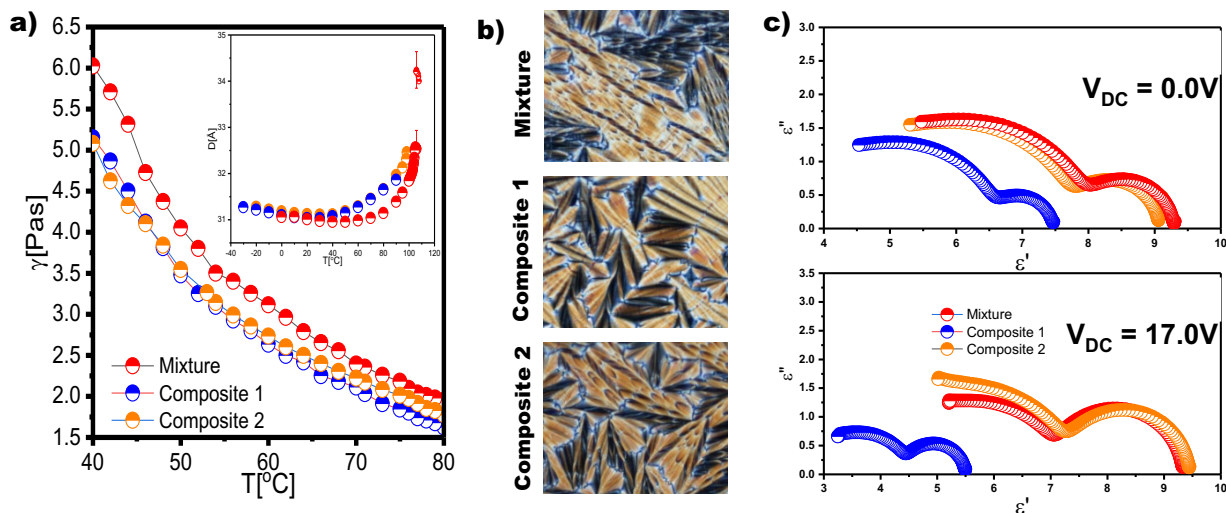


Fig. 1 Temperature dependence of the rotational viscosity and smectic layer thickness (a), optical textures registered in the SmC*_A phase (b) and Cole–Cole plots with and without bias field (d) for pure binary mixture and two composites.

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Aggregation Properties of a Chromonic Liquid Crystal

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Lyotropic chromonic liquid crystals (LCLCs) are water-based. The LCLC molecules usually have a plank-like or disk-like polyaromatic central core and two or more ionic groups at the periphery. Disodium cromoglycate (DSCG) is known as an antiasthmatic drug (“cromolyn”) and one of the most extensively studied LCLCs. In water, DSCG molecules assemble spontaneously by noncovalent interaction into anisotropic structures. When the DSCG concentration is high enough, molecular aggregates organize into a nematic liquid crystal phase with orientational order [Figure (a)]. Even for very diluted, isotropic solutions, the absorption of UV radiation depends strongly on the concentration, which may be explained by the successive formation of different assembly sizes, which exhibit different light absorption [Figure (b)]. In other LCLCs, multiple peaks in the visible absorption spectrum have been assigned to single molecules or to assemblies with different fractions of molecules, respectively [1]. The respective peaks may decrease or increase during the assembly process and may red-shift or blue-shift as the assembly structure changes. This work focuses on changes in the UV absorption spectrum of diluted and higher concentrated mesogenic aqueous DSCG solutions with increasing concentration. We try to understand the assembly process in this system.

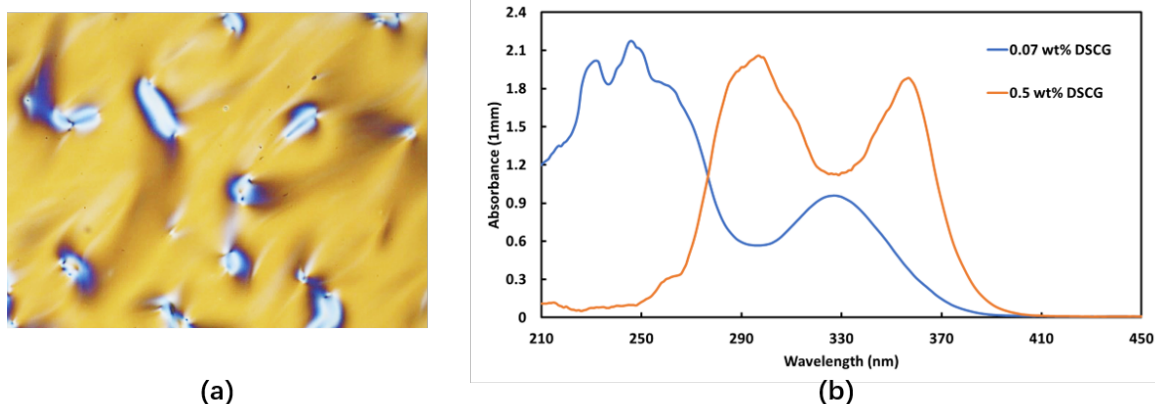


Figure (a): POM microphotographs of nematic liquid crystal phase of an aqueous solution of DSCG with a concentration of 14 wt% DSCG at room temperature. Figure (b): Absorption spectra of 0.07 wt% and 0.5 wt% DSCG in water.

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Influence of the annealing conditions and the host materials on a columnar liquid crystal based OLED

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In previous works, the columnar discotic liquid crystal (LC) perylene-3,4,9,10-tetracarboxylic tetraethylester (PTCTE), a fluorescent organic semiconductor, was found to show decent performance in an organic light emitting diode (OLED) [1-3]. The present study reveals that the luminance is affected by annealing. An enhancement of the luminance can be attributed to an improved hole injection [4]. Annealing at 120 °C leads to a higher luminance and an improved EQE (**Figure 1a**). However, if the annealing temperature is too high, the luminance is found to decrease.

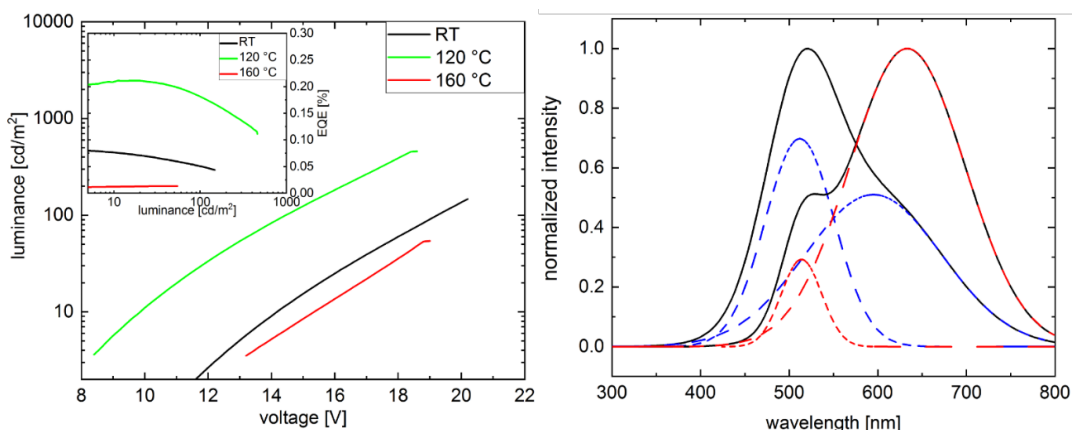


Figure 1: a) Luminance of the OLED with Spiro-TTB as hole transport layer and LiF as electron injection layer with and without annealing. The inset shows the EQE of the OLED. b) Normalized intensity of the fitted spectra (solid line) with the fitted contributions of the localized exciton and exciplex emission (dashed line, red: 3.2 V; blue: 5.0 V).

We also tried to raise the efficiency by embedding the LC in a host material. In addition to improvements of the external quantum efficiency (EQE) and the luminance of the OLED, the intensity distribution of the electroluminescence spectra was found to change, when the voltage increases (**Figure 1b**). The luminescence peaks appear at $\lambda = 668$ nm for voltages up to 3.4 V and at $\lambda = 516$ nm for voltages larger than 3.8 V. While the emission at low voltages originates from excimer formation of PTCTE [4], the latter emission (at 516 nm) can be attributed to localized excitons within PTCTE.

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Lyotropic myelin structures stained with Nile Red

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Many biologically relevant entities show unique ability to create liquid crystalline arrangement. Mesophases can be observed in complex biological systems, for instance in cell membrane and myelin sheath [1]. The well-known example of lyotropic liquid crystals is artificial myelin structure, which is formed by phospholipids multilayers in aqueous environment [2]. Stacked bilayers of amphiphilic molecules show both directional order along the hydrocarbon chains and ability to slide with respect to each other. The important advantage of myelin structure made of a single type of biomacromolecules is obtaining a simplified model of biological membrane.

In this study, we present formation and analysis of lyotropic myelin figures composed of zwitterionic phospholipids stained with Nile Red. The combination of polarized light microscopy and fluorescence confocal microscopy was used to investigate the morphology of multilayered structures. Moreover we showed spontaneous and stimulated formation of branched lipid tubes.

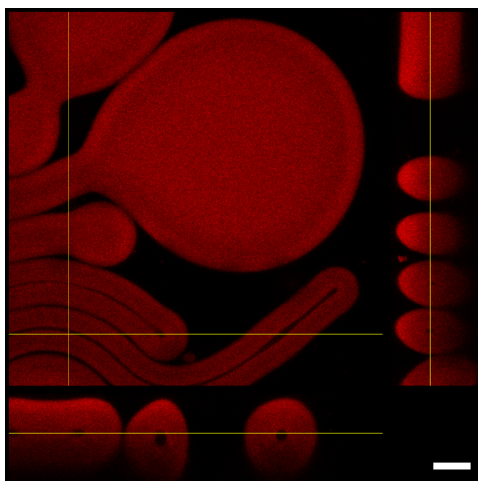


Figure 1. Confocal fluorescent image of myelin figures stained with Nile Red. Scale bar is 20 μm .

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Intermolecular proton transfer between liquid crystalline chiral 4-phenylpyridine derivative and organic acids

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Mixtures of nematic liquid crystal with chiral ionic liquids are the subject of research as they may be used to electrically control selective reflection band or to electrically induce cholesterics gratings [1, 2]. Based on our unpublished results, we noticed often poor solubility of ionic liquids in nematic hosts. We assume that synthesis of chiral ionic liquids with anion and/or cation containing a mesogen may result in good compatibility of such systems with nematic liquid crystal host.

One of the approaches which may be used to synthesize chiral ionic liquid compounds compatible with nematic liquid crystal host is to utilize the hydrogen bond between proper proton donor (acid) and proton acceptor (e.g. pyridine derivative). In such systems one or two of the components may be chiral and one or two of them may possess mesogenic group. It is believed, that in case when value of ΔpK_a , defined as difference between pK_a value of acid conjugated with the proper proton acceptor (pyridine derivative) and pK_a value of acid, is more than 3, the formation of ionic salts is promoted and co-crystal formation is expected when ΔpK_a is below 3 [3]. This parameter may be one of the measurement of proton transfer affinity.

The aim of our studies was to synthesize and characterize properties of system composed of chiral liquid crystalline 4-phenylpyridine derivative (ZW8565, mesogenic proton acceptor) and various organic acids (proton donors) differs in strength and to establish the influence of strength of acid on type of the bond being formed between ZW8565 and acid (ionic bond or hydrogen bond). The studies include mid-infrared spectroscopy, polarizing optical microscopy characterization of phases and phase transition temperatures of systems based on chiral liquid crystalline 4-phenylpyridine derivative and selected organic acids. Moreover, the compatibility of synthesized systems with nematic liquid crystal host was determined and selected examples will be presented.

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Self-Assembly of Aminocyclopropenium Salts: En Route to Deltic Ionic Liquid Crystals

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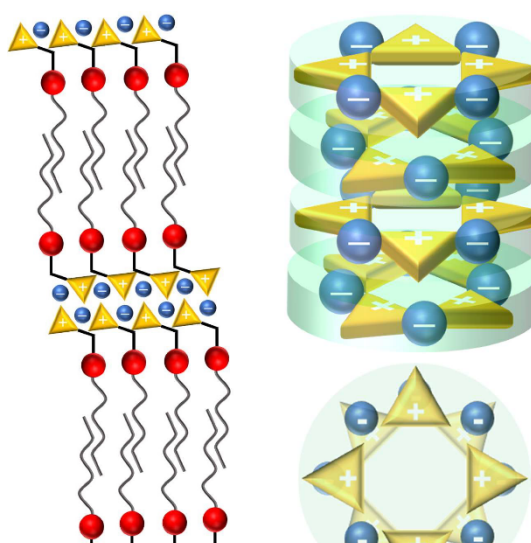
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Ionic liquid crystals [2] (ILCs) with deltic head group based on aminocyclopropenium were synthesized. These are the first examples of liquid crystalline cyclopropenium derivatives. The combination of this head group and a small core with one alkoxy chain led to bilayered smectic mesophases. An extended core with three alkoxy chains and the same head group gave columnar mesophases. The combination of a more sterically demanding aminocyclopropenium headgroup with the same core resulted again in a smectic mesophase, however.

Grafting two cyclopropenium groups at the head of one molecule led to a non-mesomorphic compound.

We compared several derivatives with the corresponding guanidinium salts. The guanidinium group has a very similar size as cyclopropenium head group. The same type mesophase with similar phase transition temperatures were observed.

Hence, we observed a dependence of the mesophase geometry from the effective volume of the head group compared to the effective volume of hydrophobic parts.



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Figure 1 - Proposed packing models of the observed mesophases. Smectic A_d phase with double layers (left) for derivatives with one alkyl chain or huge steric demand of cyclopropenium head group. Columnar mesophase from side (top right) and top view (bottom right) for derivatives with three alkyl chains and less steric demand of cyclopropenium head group. Figure

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Induction of smectic A phase in mixtures of nematic compounds showing positive and negative dielectric anisotropy

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The results of miscibility studies of compounds showing positive and negative dielectric anisotropy will be presented. The first group of compounds contain $-\text{OCF}_3$ and $-\text{NCS}$ terminal groups, the second group of compounds contain alkyl or alkoxy groups in terminal position as well as fluorine atoms in lateral positions. The tested compounds do not form smectic A phase but this phase appears in their mixtures. The phase diagrams of mixtures as well as results of calculations of the lengths of molecules and molecular cores, parallel and perpendicular dipole moments and polarizabilities of investigated compounds, calculated with the use of Scigress software, will be presented. The influence of the compounds structure on temperature and concentration range of the induced smectic A phase will be shown.

Odd-even effect in homologous series of 4-cyano-3-fluorophenyl 4'-*n*-benzoates (*n*CFPB)

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Learning thermodynamic properties and the analysis of the associated changes to the dynamics, e.g. vibrational modes, allowed us to determine the phase diagram of individual homologues of the series of 4-cyano-3-fluorophenyl 4'-*n*-benzoates (chemical formula $C_nH_{2n+1}-C_6H_4-COO-C_6H_3F-CN$, abbreviated *n*CFPB) for $n = 3 - 9$. The results of complementary measurements of *n*CFPB will be presented. Moreover, *ab-initio* simulations showed how CFPB molecules are arranged in ordered phases (examples are shown in Fig. 1).

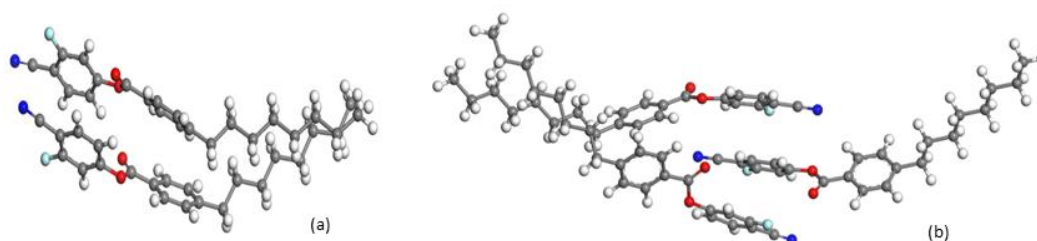


Fig. 1. Clusters of (a) dimer and (b) trimer of 8CFPB molecules.

Polymorphism strongly depends on the length of the hydrocarbon chains as well as the rate of temperature changes. Rotation of chain fragments is active in long chains, and in crystal phases (ODIC or CONDIS) as well as in liquid crystal mesophases, see Fig. 2.

Molecules of *n*CFPB have one fluorine atom, substituting hydrogen in the phenyl ring. Fluorine substitution for one or more H atoms in such structures results in an interesting behaviour of the compounds [1,2]. For instance, the clearing temperature of 5CFPB ($n = 5$) is by 30°C lower than the corresponding un-fluorinated compound. However, a substitution of the other hydrogen atoms by the fluorine atoms in the molecules of this series leads to only 1°C difference between the melting temperatures, whereas the nematic – isotropic liquid transition temperatures are lowered by about 30% [3]. Moreover, fluorine substitution results in a higher chemical stability of the modified compound and its lower viscosity. These modifications of physical and chemical properties are of interest to the material engineers seeking materials suitable for particular industrial applications.

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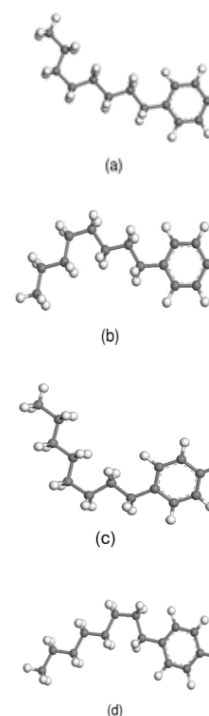


Fig. 2. Possible conformations of tail group of 8CFPB.

Electric conductivity and electric polarisation of electrodes as markers of phase transitions

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Broadband Dielectric Spectroscopy allows one to study dielectric relaxation of disordered systems, comprising polar molecules with some degrees of reorientational freedom, i.e. a gradual return of a system to its equilibrium state after removal of the external disturbance, as the electric field. In general at selected temperature, one registers complex dielectric spectra in any thermodynamic phases, i.e. from the dielectric response one gets information about contributions to the dielectric permittivity from: relaxation process (or processes) $\varepsilon_{R.P.}^*(\omega)$, electric conductivity $\sigma'(\omega)$ and, in some cases, electrode polarization of electrodes $B'(\omega)$ [1-4]. The real part of the electric conductivity (contributing to the imaginary part of dielectric permittivity by $\varepsilon''(\omega) = \sigma'(\omega)/\epsilon_0\omega$, where ϵ_0 is the permittivity of the vacuum) does not depend on the frequency (is constant) and its imaginary part equals zero for the ohmic electric conductivity. For non-ohmic conductivity the electric conductivity depends on the frequency and then, in general, one gets that the contribution from the electric conductivity to the imaginary part of the permittivity is a power function of frequency with an exponent n , for $0 < n \leq 1$ [3,4]. The electrode polarisation is an unwanted effect during dielectric experiments. At low-frequencies the real part of the dielectric permittivity increases with decreasing frequencies. The molecular origin of the electrode polarisation is a partial or a whole blocking of charge carriers at the interface between the sample and electrode areas. In a consequence, it leads to a separation of positive and negative charges giving a rise to an additional polarisation and, at the same time, lowering the electric conductivity in the low-frequency region. Then, in general, the contribution to the real part of the dielectric permittivity from the electrode polarisation is described by a power law of the frequency with an exponent m , for $0 \leq m \leq 2$ [3,4]. It will be shown that the exponents n and m take the appropriate values depending on a thermodynamic phase. Thus, they are excellent markers of phase transitions, and they can help 'identify' thermodynamic phases. Analyses will be presented for various phases of different liquid crystals.

Acknowledgments. The work was partially supported by the Polish-Italy bilateral joint research project for years 2020 – 2021 “*Multidisciplinary studies of glass-forming molecular materials*”, and the funding from the JINR (Joint Institute of Nuclear Research, Dubna, Russia) research group and centres in Poland – project “*Studies of selected soft materials and compounds in nanoporous materials*”.

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Can Onsager theory describe smectic liquid crystals ordering?

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For a long time there was a widespread belief that the Onsager theory (OT) [1] can only be applied to describe nematic liquid crystal phases (LCs) of very elongated hard molecules that exhibit no density changes and that it is of no use in the case of the smectic phase formation. With passing the time it became clear that it also works for molecules with smaller aspect ratio (length-to-width ratio) and occurring discrepancy in prediction the phase transition points from the isotropic to the nematic phase can be reconciled with the simulation outcome by using, for instance, the Parsons-Lee density scaling [2]. Next, it occurred that OT can be also successfully applied to the structure of a liquid crystal confined to a slit [3,4,5]. Here, application of the Gaussian quadrature integration scheme to estimate integrals in OT [6] has allowed to obtain not only orientational order profiles but as well as the density changes. Also the Parsons Lee scaling provided a good comparison between simulations and theory. More work and references on this topic one can find in [5].

An interesting thing was that the confined LC system with density changes was an easier problem to solve than the bulk spatially modulated smectic phase. The problem with finding solution to the OT theory arises mainly from multidimensional integrals that are inherent to the OT theory, which require high accuracy in their calculations.

Recently an efficient scheme has been proposed how to calculate density profiles in infinite, modulated and perfectly aligned two-dimensional systems of boomerangs [7,8], which may form, upon reaching appropriate density, ferroelectric or antiferroelectric smectic ordering. Similar idea of perfectly aligned LC systems has been also used by other researchers [9].

In the current work we have undertaken an attempt to solve the OT theory of a two-dimensional system of fused spheres from which rods of different lengths can be created, with possibility to rotate. To assess applicability of the OT theory the outcome will be compared to the simulation data from molecular dynamics performed with the help of LAMMPS.

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Charge transport properties in hybrid discotic matrix amalgamated with 0D nanostructured materials

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Triphenylene core based discotic liquid crystals have proven their potential for modern optoelectronic devices due to their high charge carrier mobility of the order of 10^{-1} to 10^{-3} $\text{cm}^2\text{V}^{-1}\text{s}^{-1}$ [1,2]. These discotic LCs commonly exhibit hexagonal columnar (Col_h) phase via π - π stacking of the molecules. In the Col_h phase, molecules align homeotropically i.e. oriented parallel to the substrate in which 1D charge transport takes place via hopping mechanism. Herein, we present the charge transport mechanism in the triphenylene-core grafted 2,3,6,7,10,11-hexabutyloxytriphenylene (HAT4) discotic mesogens along with their composites made with Carbon dots of size 7–8 nm. The triphenylene matrix remains invariant after the controlled dispersion of quantum sized C-dots; nevertheless, the electronic and transport properties of the neat matrix have been changed significantly. The percolated network of C-dots in the HAT4 matrix offers 102 times higher conduction current in the columnar phase; however, the charge carrier mobility is found to be lowered due to the change in the columnar ordering. The superior electronic behavior of the HAT4/C-dot composites could overcome the poor conductivity of organic semiconductors and hence, it is suitable for organic semiconducting devices and optoelectronics.

- [1] A. Gowda et al., *ChemistrySelect*, **3**, 6551– 6560, (2018).
- [2] P. Mahesh, *J. Mater. Chem. C*, **8**, 9252–9261, (2020).

Temperature-induced liquid crystal microdroplets and templated microparticles in a partially miscible liquid mixture

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Liquid-in-liquid droplets are typically generated by the partitioning of immiscible fluids, e.g. by mechanical shearing with macroscopic homogenisers or microfluidic flow focussing. In contrast, partially miscible liquids display a temperature-dependent mixing behaviour. We have investigated this phenomenon for a liquid mixture composed of methanol (MeOH) and the thermotropic liquid crystal 4-Cyano-4'-pentylbiphenyl (5CB). A temperature induced phase separation upon cooling leads to nucleation, growth and coalescence of mesogen-rich droplets. The number of nucleation points and size of isotropic and nematic droplets over time can be tuned on a microscopic scale by variation of temperature quench depth and cooling rate. Liquid crystal droplets in the nematic phase adopt a radial configuration, with interesting topological transformations.¹

Further, we have explored the potential of this system to be utilised for the production of polymeric microparticles. Non-reactive 5CB was mixed with the reactive mesogen 2-methyl-1,4-phenylene bis{4-[3-(acryloyloxy)propoxy]benzoate} (RM257) before mixing with methanol. Well-defined droplets were formed by temperature-induced phase separation with ensuing photopolymerisation via the exposure of RM257 to UV light. Subsequent heating of the mixture led to the diffusion of unreacted 5CB back into the methanol phase, separating the 5CB-MeOH liquid mixture from the formed polymer.² The use of a reversible materials templating approach for an irreversible polymer product has relevance in diagnostics, optoelectronics and extraction processes.

- [1] M. Patel, A. N. P. Radhakrishnan, L. Bescher, E. Hunter-Sellars, B. Schmidt-Hansberg, E. Amstad, S. Ibsen and S. Guldin, *Soft Matter*, **17**, 947 – 954 (2021).
[2] M. Patel, A. Taylor and S. Guldin [In progress]

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Complex dynamics and phase behaviour of liquid crystals under pressure

Participants and Presentations

Name	Affiliation	Label	Time
Abele, Christina	University of Stuttgart	O20	Fr 13:00
Alaasar, Mohamed	MLU-Halle	O17	Fr 11:00
Ali, Muhammad	University of Warsaw, Faculty of Chemistry	O1	We 9:30
Araoka, Fumito	Tokyo Institute of Technology	I1	We 9:00
Baumann, Maximilian	University of Würzburg	S14/P14	We 16:25
Becker, David	Universität Paderborn	S38	Th 14:35
Belyaev, Victor	Moscow Region State University	S29/P29	Th 11:50
Benkowska-Biernacka, Dominika	Wroclaw University of Science and Technology	S39	Th 14:40
Blanke, Meik	Universität Duisburg-Essen	O8	Th 9:30
Brecht, Berteloot	ELIS Department, Ghent University	O4	We 14:30
Bruckner, Johanna	University of Stuttgart	S30/P30	Th 11:55
Busch, Mark	Hamburg University of Technology	S33	Th 12:10
Černá, Tereza	University of Chemistry and Technology Prague	S07/P07	We 12:00
Chrzanowska, Agnieszka	Kraków University of Technology	S45	Th 15:10
Dardas, Dorota	Polish Academy of Sciences Poznan	S28/P28	Th 11:45
Deptuch, Aleksandra	Polish Academy of Sciences Kraków	S22/P22	We 17:05
Dieterich, Sonja	University of Stuttgart	O14	Fr 9:00
Drzewicz, Anna	Polish Academy of Sciences Kraków	S21/P21	We 17:00
Duda, Łukasz	PORT Polish Center for Technology Development	S40	Th 14:45
Ebert, Max	Universität Stuttgart	S41	Th 14:50
Filimonova, Evgeniia	MLU-Halle	S23/P23	We 17:10
Fryń, Paryk	Jagiellonian University Kraków	S08/P08	We 12:05
Galazka, Mirosław	Polish Academy of Sciences Kraków	S44	Th 15:05
Geivandov, Artur	FSRC Crystallography and Photonics RAS Moscow	O15	Fr 9:20
Gerbis, Lisa	University of Würzburg	S06/P06	We 11:55
Godinho, Helena	Universidade NOVA de Lisboa	I8	Fr 13:40
Görtz, Verena	Lancaster University	V2	Th 19:30
Grunwald, Marco	Universität Stuttgart,	S19/P19	We 16:50
Habibpourmoghadam, Atefeh	OvGU Magdeburg/Uni Paderborn	O6	We 15:10
Haage, Christian	University of Stuttgart	S10/P10	We 12:15
Herzog, Anselm	University of Würzburg	S12/P12	We 12:25
Honaker, Lawrence	Wageningen University	O2	We 9:50
Ignés-Mullol, Jordi	Universitat de Barcelona	I3	We 14:00
Ivanov, Viktor	MLU-Halle	S15/P15	We 16:30
Jakli, Antal	Liquid Crystal Institute, KSU, Kent, OH	Saupe	Th 18:00
Jasiurkowska-Delaporte, Małgorzata	Polish Academy of Sciences Kraków	O12	Th 16:20
Juszyńska-Gałązka, Ewa	Polish Academy of Sciences Kraków	S43	Th 15:00
Kasyanova Irina	Russian Academy of Sciences	S27/P27	Th 11:40
Kitzerow, Heinz	Paderborn University	S03/P03	We 11:40

Klopp, Christoph	Otto von Guericke University, Magdeburg	S02/P02	We 11:35
Klopp, Christoph	Otto von Guericke University, Magdeburg	S20/P20	We 16:55
Lalik, Sebastian	Jagiellonian University Kraków	S36	Th 12:25
Lambov, Martin	University of Wuerzburg	O9	Th 9:50
Lesiak, Piotr	Warsaw University of Technology	O19	Fr 11:40
Loiko, Valery	Institute of physics of NAS Belarus Minsk	S05/P05	We 11:50
Maaß, Corinna	Max Planck Institute, Göttingen	I5	Th 11:00
Malotke, Florian	Universität Duisburg-Essen	O7	We 16:00
Mamuk, Atilla Eren	Mugla Sitki Kocman University, TURKEY	S31/P31	Th 12:00
Menzel, Andreas	Otto von Guericke University, Magdeburg	V1	We 19:30
Mertelj, Alenka	Jožef Stefan Institute, Ljubljana	I7	Fr 10:30
Nath, Subrata	Universität Duisburg-Essen	O10	Th 10:10
Noll, Katja	Universität Würzburg,	S09/P09	We 12:10
Nordendorf, Gaby	Paderborn University	S26/P26	Th 11:35
Novotna, Vladimira	Czech Academy of Sciences, Praha	I4	Th 9:00
Patel, Mehzabin	University College London	X47	Th 15:20
Perkowski, Paweł	Military University of Technology, Warsaw	S18/P18	We 16:45
Pieranski, Paweł	Université Paris-Saclay	O21	Fr 13:20
Piowarczyk, Marcin	Polish Academy of Sciences Kraków	S24/P24	We 17:15
Prasad, Aparna	University of Würzburg	S16/P16	We 16:35
Ramou, Efthymia	NOVA University of Lisbon,	S25/P25	Th 11:30
Raszewski, Zbigniew	Military University of Technology, Warsaw	S34	Th 12:15
Ravnik, Miha	University of Ljubljana	I6	Th 14:00
Rybak Paulina	University of Warsaw	O18	Fr 11:20
Scheuring, Nikolai	University of Würzburg	S11/P11	We 12:20
Schmidtke, Jürgen	Paderborn University	S04/P04	We 11:45
Selvaraj, Pravinraj	National Changhua University of Education	O13	Th 16:40
Sharma, Anjali	University of Luxembourg	O3	We 10:10
Shvetsov, Sergey	Lomonosov Moscow State University	O5	We 14:50
Simdyankin, Ivan	FSRC Crystallography and Photonics RAS Moscow	S01/P01	We 11:30
Singh, Dharmendra Pratap	Université du Littoral Côte d'Opale (ULCO)	S46	Th 15:15
Šmahel, Michal	University of Chemistry and Technology, Prague	S17/P17	We 16:40
Starzone, Szymon	Polish Academy of Sciences	X50	Th 15:25
Stebryte, Migle	ELIS department, Ghent University	S32/P32	Th 12:05
Tomczyk, Wojciech	Jagiellonian University Kraków	O16	Fr 9:40
Tykarska, Marzena	Military University of Technology Warsaw	S35	Th 12:20
Walker, Rebecca	University of Aberdeen	I2	We 11:00
Weinberger, Pascal	Universtiy of Würzburg	S13/P13	We 16:20
Zavvou, Evangelia	University of Patras	O11	Th 16:00
Zhang, Bingru	Paderborn University	S37	Th 14:30
Zieja, Paulina	Military University of Technology Warsaw	S42	Th 14:55