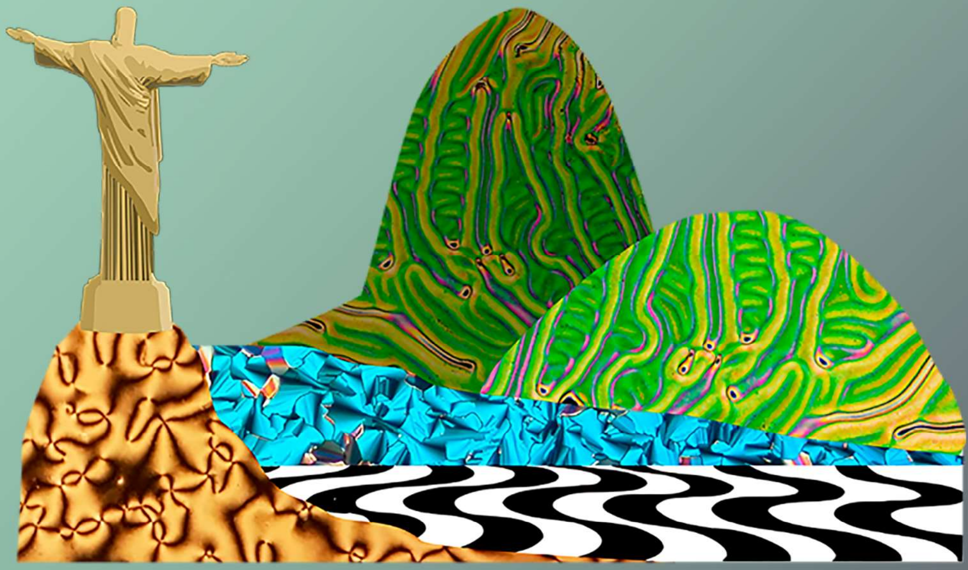

ILCC - 2024

Rio de Janeiro -Brazil

Proceedings

HUGO GALLARDO
IVAN H. BECHTOLD

Proceedings of the 29th International Liquid Crystal Conference

Rio de Janeiro-RJ
2024

Revisão textual e gramatical: Resposanbilidade dos respectivos autores.

Dados Internacionais de Catalogação na Publicação (CIP)
(Câmara Brasileira do Livro, SP, Brasil)

International Liquid Crystal Conference (29. : 21-26 jul. 2024 : Rio de Janeiro, RJ)
Proceedings of the 29th International Liquid Crystal Conference [livro eletrônico] / Hugo Gallardo, Ivan H. Bechtold. -- Rio de Janeiro : Aptor Software, 2024.
PDF

Vários autores.
Bibliografia
ISBN 978-85-63273-60-4

1. Congressos 2. Cristais 3. Química I. Gallardo, Hugo. II. Bechtold, Ivan H. III. Título.

24-222623 CDD-540

Índices para catálogo sistemático:

1. Química 540

Eliane de Freitas Leite - Bibliotecária - CRB 8/8415

Foreword

Dear Friends and Colleagues,

The 29th Edition of the International Liquid Crystal Conference (ILCC 2024) was held for the first time in Latin America, from July 21st to 26th, 2024. Brazil was chosen to host this important event due to its importance and relevance in the field of liquid crystals. In addition, Rio de Janeiro with its unparalleled natural beauty, is a city full of history and very friendly people.

The organizing committee was dedicated to encouraged students, young researchers and women to participate, considering the importance of new generations and women representation in the International Liquid Crystal Society (ILCS). 35 different countries were represented, consisting of 34.6% women, 65.1% men and 0.3% others, and encompassing 62.3% professionals and 37.7% students. Women were 37% of the invited speakers and 31% were young researchers.

The ILCC 2024 was a great success thanks to your participation and communications, being a stage for science discussions and collaborations related to liquid crystals, their fundamentals, novelties, applications and trends.

Thank you very Much! (Muito obrigado!)

ILCC 2024 Organizing Committee.

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Summary

A Design, Synthesis and Characterization

B Macromolecular Liquid Crystals

C Ferroelectric materials

D Novel Applications

E Liquid Crystals in Biology, Circular Economy, Sustainability

F Mathematical Modeling, Symmetry and Topolgy

Plenary Lecture

Active nematics: A new approach to mechanobiology?

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Keywords: active nematics, active turbulence, topological defects, mechanobiology, gastrulation

Active materials such as bacteria, molecular motors and eukaryotic cells continuously transform chemical energy taken from their surroundings to mechanical work. Dense active nematics show mesoscale turbulence, the emergence of chaotic flow structures characterised by high vorticity and self-propelled topological defects. I shall describe the physics of active nematics and discuss how this may be relevant to biological processes such as cell sorting and early embryogenesis.

Advanced Functional Liquid-Crystalline Materials

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Keywords: Liquid Crystal, Self-Organization, Nanostructure, Supramolecular Assembly

Supramolecular self-assembly of liqiud-crystalline (LC) molecules has attracted much attention because a varitey of advanced functions of transport, information, sensing, acturation, photofunction, and biofunctions can be induced due to these dynamic and self-organized structures. Design of molecular structures and control of molecular interactions are the key to obtain highly functional LC nano-assemblies.[1-7] Here nanostructured functional LC materials are presented in view of design and self-organization of 1D, 2D, and 3D nanostructures. Collaboration of materials design with molecular dynamics (MD)[3,8,9] simulation and advanced measurements[10,11] are also described. For example, smectic LC materials have been applied to 2D nanostructured electrolytes[7,12] and water treatment membranes[3,13]. Stable behavior as lithium ion batteries was observed for the 2D LC electrolytes.[7,12] High virus removal was achieved for nanostructured polymers preserving 2D smectic structures derived from phase segregation.[3,13] Relationships of 1D, 2D, and 3D nanostructures and their advanced functions have been studied by MD simulation and X-ray spectroscopy.[8,9,10,11] For example, 2D phase structures and their transitions of smectic electrolyte moleules are well explained by the results with electron-density maps obtained by X-ray and MD simulations.[9] Moreover, selective properties of subnanoporous water treatment LC membranes have been well explained by soft X-ray emission study of the synchrotron facilities.[11] Liquid crystals have great potential as highly functional soft matter in a variety of fields based on nature of self-organized dynamic structures.

Acknowledgements: Financially supports of KAKENHI JP19H05715, JST-CREST JPMJCR1422, JPMJCR20H3, and MEXT Material R&D project JPMXP1122714694 are gratefully acknowledged.

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Polar Order in Liquid Crystals

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Polar molecules are ubiquitous in our daily lives (e.g. water), possessing regions of positive and negative charges that generate a permanent electric dipole moment. While these dipoles are usually randomly oriented and cancel out in condensed phases, the ferroelectric nematic phase (NF) is an exception; the constituent molecular dipoles align parallel to each other, resulting in a bulk material that is polar. [1-7] In just a few years the NF phase has transitioned from being a curiosity found only in one or two materials (RM734, DIO), to being an established area of LC science.

The NF phase is just one example of a LC phase that exhibits polar order. In this talk, I will outline our ongoing work at the University of Leeds that focuses on new materials design and development allied to predictive simulations and calculations, the discovery of new polar phase types, and our development of room temperature NF materials.

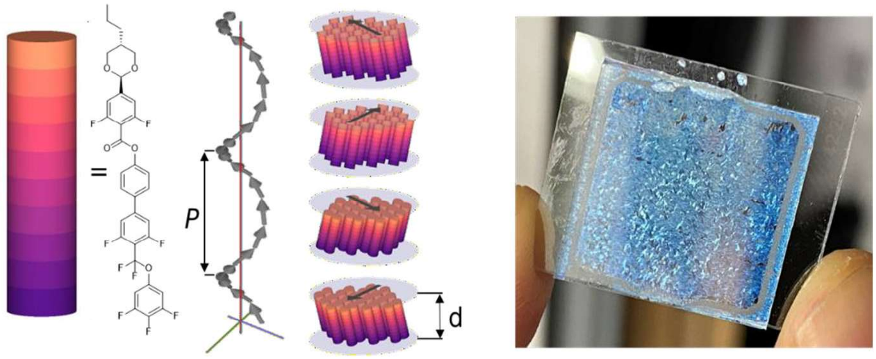

Fig. 1: Proposed structure of a helical polar smectic C variant discovered at the university of Leeds (left), which displays selective reflection (right) and operates at sub ambient temperature. [7]

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Spontaneously polar or/and twisted liquid crystal structures

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Keywords: polar nematics, chirality, twist-bend phases

In nature, helical structures are widespread and manifest across a range of scales, spanning from nanometres to macro scales. Helices are often formed by biological polymers, such as DNA or collagen, and their formation is attributed to the twisted assemblies of chiral molecules, stemming from the asymmetry in the arrangement of neighboring components. However, it is noteworthy that helices are not exclusively linked to molecular-level chirality.

Liquid crystals, specifically the twist-bend phases (nematic and smectics), composed of achiral bent dimers or rigid bent-core molecules, have been recognized for several years. The short helices observed in these phases are attributed to a reduction in bend elasticity resulting from the distinctive molecular shape. While the twist-bend nematic phase exhibits a relatively simple structure with a single short helix, smectic phases have been observed to form a double helix, with a longer helix superimposed on a shorter one [1]. Also more intricate multi-helical structures have been identified.

Our recent research has unveiled also a ferroelectric analogue of the N_{TB} (polar twist-bend) phase, comprising molecules with strong dipole moments [2].

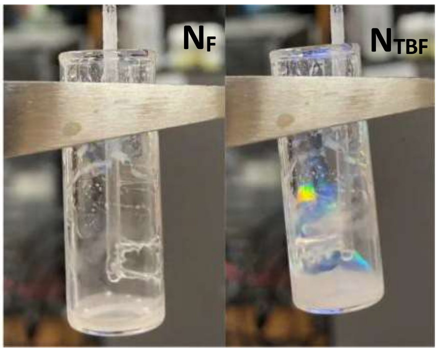

Fig. 1 Phase transition form N_F to helical N_{TBF} phase

The spontaneous helix in the polar N_{TB} phase is significantly longer than in its apolar counterpart, resulting in selective light reflection in the visible range (Fig. 1). Despite its similarity to the heliconical non-polar twist-bend nematic phase, the genesis of this novel liquid crystalline phase differs. It emerges due to electrical interactions that induce a non-collinear orientation of electric dipoles, resembling the observed behavior of spins in magnetic systems. Considering that the Dzyaloshinskii-Moriya interaction generates a diverse array of chiral topologies in magnetic spins, such as helical or skyrmion phases, one may pose the question of whether an analogous interaction of electric dipoles may lead to similar structural complexity.

Acknowledgements: The research was supported by the National Science Centre (Poland) under the grant no. 2021/43/B/ST5/00240 and by Military University of Technology under research project UGB 22-801.

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Stimuli-Responsive Liquid Crystalline Materials: From Tunable Photonics to Deformable Soft Systems

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Keywords: Stimuli-Responsive, Liquid Crystal, Tunable Photonics, Deformable Soft System

Liquid crystals (LCs) represent a fascinating state of matter that combines order and mobility on a molecular and supramolecular level. The unique combination of order and mobility results in that LC is typically “soft” and responds easily to external stimuli. The responsive nature and diversity of LCs provide tremendous opportunities as well as challenges for insights in fundamental science, and open the door to various applications. Conventional nematic LCs have become the quintessential materials of LC displays. With the LC displays ubiquitous in our daily life, the research and development of LCs are moving rapidly beyond display applications and evolving into entirely new and fascinating scientific frontiers. In my talk, I will focus on our recent research and development on stimuli-responsive liquid crystalline materials: from tunable photonics to deformable soft systems.

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Tutorials

Characterisation of liquid crystals via textures: from polarising microscopy to machine learning

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Keywords: polarizing microscopy, textures, defects, Voronoi patterns, machine learning

In this tutorial we will discuss a range of methods to characterize liquid crystal phases by their textures. Starting with polarizing microscopy we will show the most characteristic textures of various different phases from nematic to smectic and soft crystals and explain some of their characteristic appearances and defects [1]. Similarly, we will shortly introduce chirality and demonstrate how novel phases such as Blue Phases and Twist Grain Boundary Phases may appear with novel and different textures and defects.

After illustrating how we can verify the structure of some liquid crystal defects [2,3], we will proceed to a short comparison with solid state systems, which often show similar defects as liquid crystals but on a very different length scale. In this context it is also demonstrated that many liquid crystal textures can in fact result from growth via a rather universally employed algorithm called Voronoi diagrams, leading to Voronoi textures [4,5].

At last, we will explore how far modern machine learning algorithms like convolutional networks and inception models can be employed to characterize liquid crystals. A range of examples will be presented from simple transitions involving the nematic phase to more complicated scenarios involving nematic, fluid smectic, and hexatic smectic order [6], and even soft crystal phases. Also, complete phase sequences in chiral liquid crystal with paraelectric, ferroelectric, ferri-, and antiferroelectric phases will be demonstrated to be predictable by machine learning [7]. Advantages and disadvantages of machine learning will be discussed, also in sight of traps to avoid [8].

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Liquid Crystal Industry Post Displays

Bahman Taheri

Alphamicron – USA

The liquid Crystal display industry has undergone a significant change over the past decade. Its exponential growth was followed by market saturation and commoditization of LCD products. This, in turn, has had a profound effect on the science and technology in this field. In this tutorial we examine how to navigate this industry by exploring other potential market sectors that can utilize unique characteristics of liquid crystals. Emphasis will be placed on use of guest-host systems for Augmented reality, Transportation, and architectural applications.

Liquid crystals as organic electronic materials

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Keywords: charge carrier transport, mobility, time-of-flight, organic transistor

Liquid crystals are interesting materials not only for display application but also electronics application. The nature of self-organizing molecular aggregation of liquid crystals are very important as organic semiconductor materials because the charge carrier transport in organic semiconductors was controlled by the molecular alignment and order. In my tutorial talk, I will show the fundamentals of electronic properties and charge carrier transport in organic semiconductors and overview the research for charge carrier transport properties and organic electronics devices in liquid crystalline materials.

Charge carrier transports in discotic and smectic liquid crystals were mainly investigated by time-of-flight technique. The electronic transport in a columnar hexagonal liquid crystal phase was revealed and the mobility show 10^{-3} cm^2/Vs in 1993.[1] The electronic transport in a smectic liquid crystal material was also showed and the mobility was 10^{-3} cm^2/Vs.[2] For the charge carrier transport in liquid crystals, the purity of material are very important and impurity molecules occurs ionic transport in especially low viscosity liquid crystal phases.[3] Electronic transport was also exhibited in nematic phases of highly purified samples. Furthermore, the polycrystalline thin film *via* liquid crystal phases showed high mobility over 0.1 cm^2/Vs, which indicated the controllable grain boundaries directions by the molecular alignment and anisotropy crystal growth.[4] Otherwise, grain boundary seriously damages charge carrier transport in non-liquid crystalline materials. Thus, liquid crystalline materials can be used in both liquid crystal phase and crystal phases.

I will also talk about liquid crystalline materials for organic electronic device such as organic transistor, organic light emitting diode, and organic solar cells. In organic transistors, the mobility is very important parameter, so crystalline small molecule and conjugated polymer materials are mainly used because the molecular order is high in crystal phases.[5,6] Liquid crystalline materials play an important role in solution fabrication process because it is possible to fabricate uniform thins films via uniform liquid crystalline thin films. The crystal phase of liquid crystalline phenyl-benzothienobenzothiophene derivative showed very high mobility over 5 cm^2/Vs and small variation.[7]

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Normal and anomalous diffusion models for the electrical impedance of liquid crystalline materials

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Keywords: Diffusion, Impedance, Liquid Crystals, Fractional Calculus

The impedance spectroscopy technique involves applying an oscillating electric field at different frequencies to a sample [1]. The impedance response of the sample provides information about various physical parameters, such as ionic motion, adsorption-desorption coefficients, viscosity, molecular polarization, conductivity, and growth dynamics [2]. The Poisson-Nernst-Planck (PNP) diffusing model, particularly its extension PNPA (anomalous), formulated using fractional calculus, has been shown to be a robust approach to interpreting impedance data in soft matter. Unlike the Warburg diffusion model, PNPA simultaneously satisfies the fractional diffusion equation and Poisson's equation, offering more reliable results.

The focus of the tutorial is thus on using impedance spectroscopy connected to the PNPA model to study ionic diffusion in soft matter, in general, and in cholesteric and modulated liquid crystal materials, in particular [3]. The model uses fractional derivatives to measure diffusivity rather than examining conductivity directly at low frequencies. Fractional calculus has been shown to be a valuable conceptual and formal tool to handle an entire class of problems [4,5]. For this reason, in this tutorial, we review the main fractional tools to formulate a diffusive model in terms of time-fractional derivatives and apply it to investigate the impedance spectroscopy of nematics, cholesterics, and other modulated phases of liquid crystals (like the twist-bend ones) in the framework of the PNPA model and anomalous diffusion behavior [6], aiming to characterize the physical parameters and diffusivity from the conductivity at low-frequency regimes [7].

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Recent Advances of Ionic Liquid Crystals

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Keywords: Ionic liquid crystals, mesophases

Ionic liquid crystals (ILCs) can be considered as a joint venture of ionic liquids (ILs), i.e. organic salts with melting points below 100°C, and thermotropic liquid crystals with anisotropic physical properties [1, 2]. However, beyond merging the physical properties of two different classes of soft matter materials ILCs possess unique properties such a 1D ion conductivity. Moreover, their phase behaviour is quite different from neutral thermotropic liquid crystals due to the importance of Coulomb interactions for the liquid crystalline self-assembly. The tutorial will discuss the unique phase behaviour, structure-property relationships, design and synthesis, theoretical concepts and recent applications of ILCs [3].

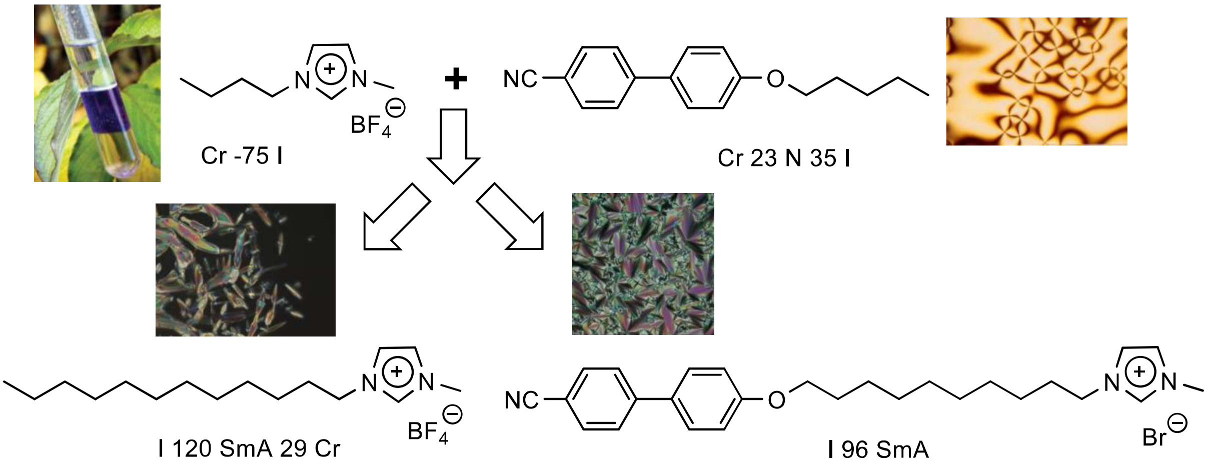

Figure 1: Tailoring the structure of IL (e.g. [BMIM]BF_4) and LC (e.g. 5OCB) results in ILCs

Acknowledgements: This work was funded by DFG (LA 907/17-2, LA 907/21-1) and DAAD -Procope (WELCHYNA).

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GB Prizes

Diffractive liquid crystal optical elements for near-eye displays

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Keywords: Liquid crystal polarization optics, near-eye display, augmented reality, virtual reality

Liquid crystal planar optics (LCPO) is emerging as a new type of optical elements with unique features like ultra-thinness, high efficiency, large angular/spectral bandwidths, polarization selectivity, and dynamic modulation [1]. In this talk, I will cover how the basic physical properties like the molecular configuration of LCPO and its optical responses are discovered and studied. The advances of fabrication techniques for future mass production and high degrees of freedom are also discussed. Finally, the applications of LCPO in near-eye displays like augmented reality and virtual reality are explored.

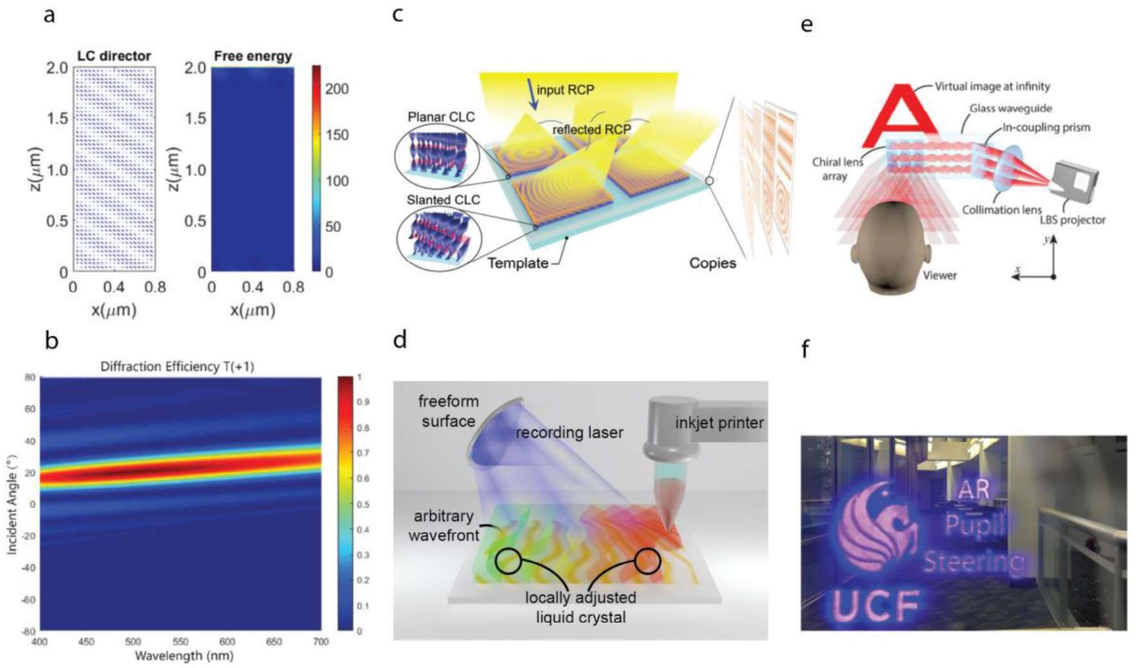

Figure 1: Outline of talk. **a** Simulation of LCPO molecular configuration. **b** Optical properties of LCPO. **c** Holo-imprinting of LCPO for mass production. **d** Full degree-of-freedom LCPO. **e** Wide field-of-view augmented reality display. **f** Pupil steering display

Acknowledgements: I would like to thank my advisor Shin-Tson Wu for the continuous support and patient guidance in my Ph.D. period.

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Electro-optics of oblique helicoidal cholesterics

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Keywords: Bragg reflection, electro-optics of liquid crystals

Absorbing materials such as pigments, inks and dyes produce colors by partially consuming the energy of light. Alternatively, colors can occur as a result of interference and diffraction of light scattered at the periodic structures with submicrometer length scales. The structural colors depend on a view angle and typically originate without energy losses which explains their widespread in Nature (bird's feathers, butterfly wings, beetles etc). The challenge is to produce mimiking materials in which the structural colors could be dynamically tuned. Among the oldest known materials capable of producing structural colors are cholesteric liquid crystals. Light causes coloration by selective Bragg reflection at the periodic helicoidal structure formed by cholesteric molecules. The cholesteric pitch and thus the color can be altered by chemical composition or by temperature, but the color tuning by electromagnetic field remains challenging. We demonstrate that a cholesteric material with a new oblique helicoidal ($\mathrm{Ch_{OH}}$) state [1-2] can produce total reflection of an obliquely incident light of any polarization [3-4]. The material reflects 100% of light within a band that is continuously tunable by electric field through the entire visible spectrum while preserving its maximum efficiency [4]. Broad electric tunability of total reflection makes the $\mathrm{Ch_{OH}}$ material suitable for applications in energy-saving smart windows, transparent displays, multispectral imaging, virtual and augmented reality.

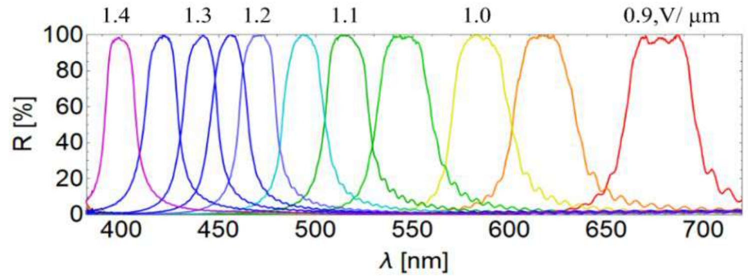

Figure 1: Electrically tunable total reflection of light produced by thin $\mathrm{Ch_{OH}}$ film, 23 μm; angle of light incidence is 45°.

Acknowledgements: NSF grants DMR-1410378, CHE-1659571 and ECCS-1906104; Mobilność Plus program (1644/MOB/V/2017/0), Kosciuszko Foundation; Oculus (Meta).

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New Phases and Phenomena of the Ferroelectric Nematic Realm

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Keywords: Ferroelectric nematic, Chiral ferroelectric nematic, Ferroelectric smectic A, Anti-ferroelectric smectic Z.

In 1916, Max Born envisioned a ferroelectric fluid in which all the dipoles point in the same direction. One century later, the ferroelectric nematic (NF) liquid crystal phase was finally found. I will present the first-principles evidence [1] for this ferroelectric nematic phase including polarization measurements which showed that the polar ordering in the NF liquid was nearly perfect, the largest ever observed in a fluid, and comparable to that of solid-state ferroelectrics. In the work that followed, three other new phases were discovered, the chiral NF with helical polar order [2], and two phases with fluid layers, the antiferroelectric SmZA [3,4], and the ferroelectric SmAF with comparable polarization [5]. The unique domain structures, defects, x-ray scattering, and electro-optic response of these phases of the ferroelectric nematic realm will be discussed.

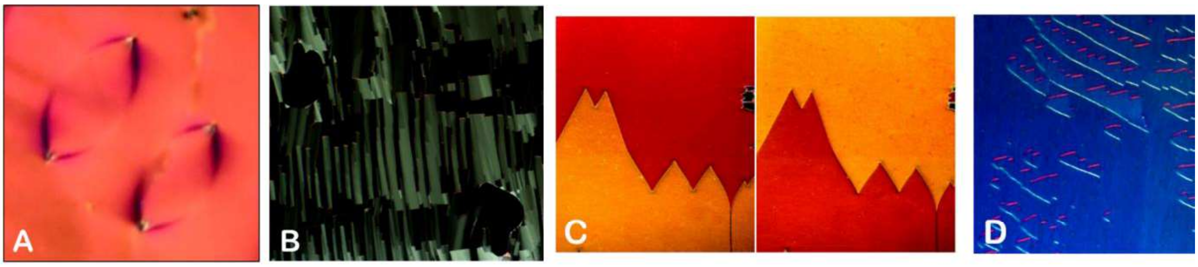

Figure 1:Ferroelectric nematic realm: (A) Ferroelectric nematic (N_F) (B) Ferroelectric smectic A (SmA_F) (C) Pi twist ferroelectric nematic (D) Anti-ferroelectric smectic Z (SmZ_A)

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Stimulus response in liquid crystalline elastomers: Fundamental characterization to functional design

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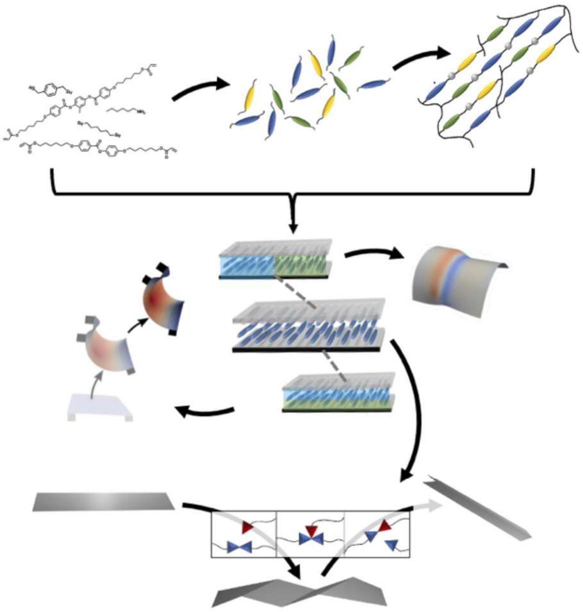

Figure 1: Fundamental liquid crystal and polymer network properties translate to functional performance and reprogrammability in liquid crystalline elastomers

Liquid crystalline elastomers (LCEs) are stimuli-responsive polymers that combine the functional properties of liquid crystals with the elastic properties of polymer networks. Reversible deformations are achieved in these materials by inducing a phase transition from the liquid crystalline mesophase to the isotropic phase, imposing a force on the polymer network connecting the mesogens. Notably, the form of deformation produced in LCEs is dependent on a combination of the global orientation of mesogens within the polymer network, phase transition temperatures, network topology, and the elastic free energy of the system. As such, it is necessary to consider mechanisms for tuning each component and understand the underlying crosstalk of these parameters.

This work demonstrates fundamental correlations between liquid crystalline phase behavior and polymer network topology as related to common alignment methods and polymerization strategies for synthesizing LCEs. [1] These relationships are then used to design complex actuations through spatial patterning of material properties to induce mechanical instabilities. [2] Finally, dynamic chemistry is leveraged to combine complex actuation modes and reprogramming modes of deformation in LCEs. [3] Overall, these studies demonstrate how manipulation and characterization of the intertwined properties of LCEs are critical to the application-driven design of LCEs as functional materials.

Acknowledgements: TSH acknowledges the Graduate Research Fellowship support from the National Science Foundation.

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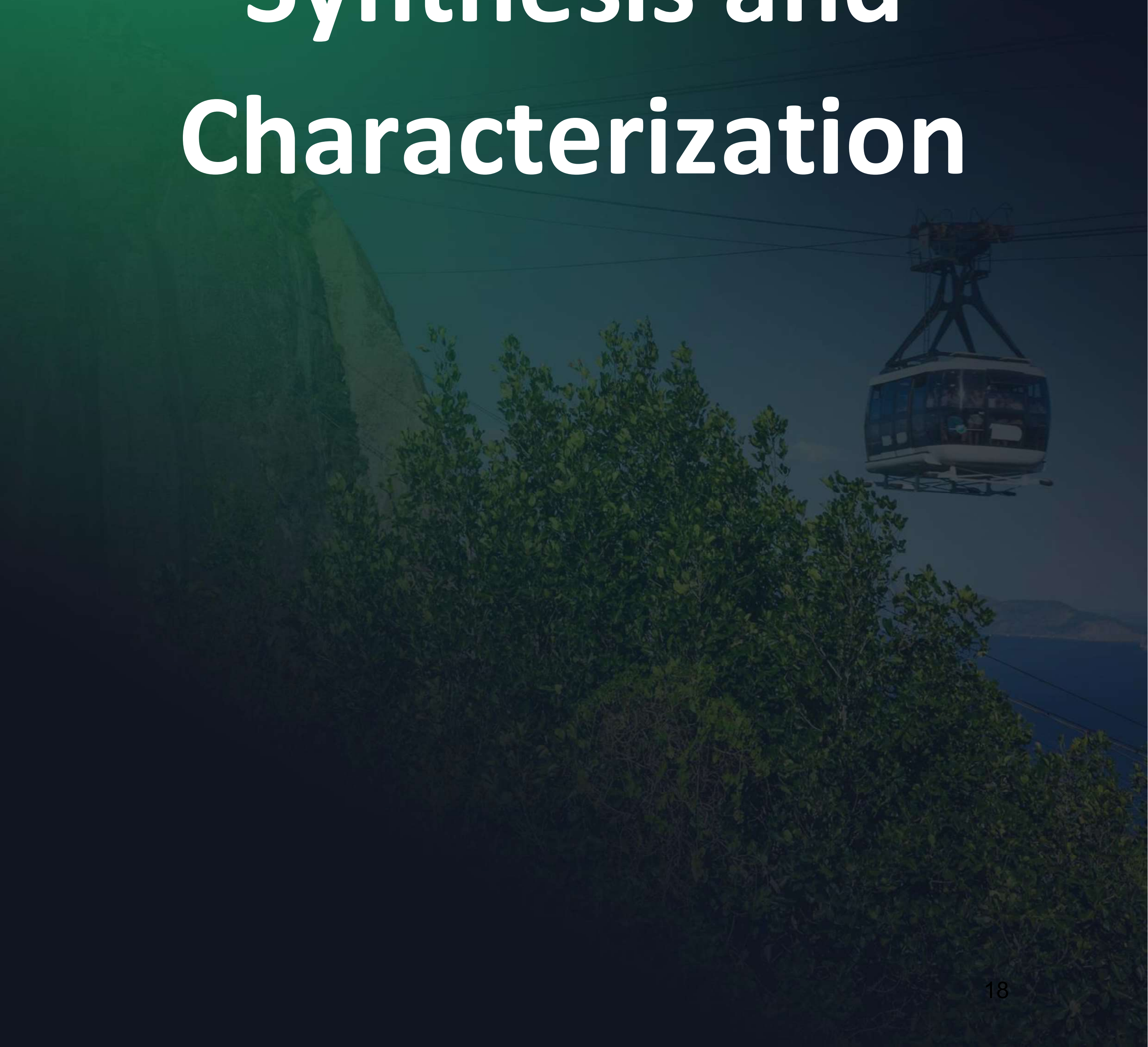
Design, Synthesis and Characterization



A1

Organic and hybrid organic materials

A novel B,O,N-doped mesogen with narrowband MR-TADF emission

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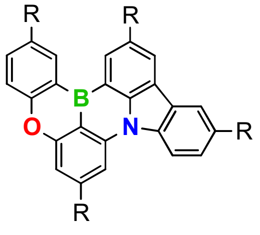
Keywords: boron, polycyclic aromatic hydrocarbons, thermally activated delayed fluorescence

Columnar self-assembly promotes enhanced charge transport in discotic liquid crystals (DLCs) which are therefore applied in (opto)electronics. Among those materials, multifaceted boron-doped polycyclic aromatic hydrocarbons (B-PAHs) have been largely neglected. Additional doping with electron-donating heteroatoms can cause antagonistic resonance effects. The resulting small singlet (S_1) and triplet (T_1) energy gap allows for multiresonance thermally activated delayed fluorescence (MR-TADF) via reverse intersystem crossing. This possibility to harvest T_1 states and the narrowband emission of such PAHs are highly sought after properties for organic light emitting diodes (OLEDs). Benefits of combination with liquid crystals like improved processability and OLED performance were recently demonstrated using a boron-free discotic nematic.[1]



BON-LC

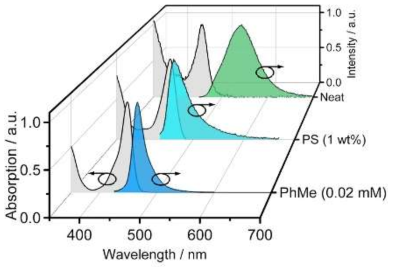


Figure 1: **BON-LC** structure, emission and absorption spectra under various conditions.

To shed light on B-PAH DLCs' great potential, an MR-TADF core motif was decorated with mesogenic groups by Suzuki-Miyaura cross-coupling yielding the first columnar MR-TADF DLC **BON-LC**. Polarized optical microscopy, differential scanning calorimetry and X-ray diffraction revealed a broad and columnar hexagonal ordered (Col_{ho}) phase. Narrowband emission from the B-PAH core and MR-TADF in doped (polystyrene matrix, 1 wt%) form were observed in photophysical investigations. Strong aggregation in the mesophase resulted in broad excimer emission without delayed component.

Acknowledgements: Studienstiftung des deutschen Volkes, DFG (INST 41/897-1, INST 41/1136-1), EPSRC (EP/P010482/1, EP/W015137/1, EP/W007517/1), LTSRF (SRF\R1\201089)

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Bent-shaped liquid crystals derived from dibenzalacetone unit

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Keywords: Bent-Shaped LCs, dibenzalacetone, dark conglomerate, bent unit.

Bent-Core Liquid Crystals (BCLCs) is still a prominent area in the liquid crystal research field due to their unique self-assembly and properties, in addition to presenting potential for new applications in smart displays and electro-optical devices, mostly because of their ability to facilitate fast switching responses.[1] This has increased the interest in the development of novel curvature core that exhibit a wide range of structural combinations. By means of this, the current work studied the applicability of a bent-core derived from dibenzalacetone (DBA) (Figure 1a, left) as a bent unit (BU) in BCLCs. This BU is intriguing due to its absence of global aromaticity while simultaneously possessing the ideal angle for bent-shape liquid crystals and a prominent transverse dipole moment generated by the carbonyl group.[2] In light of that, five new molecules containing the dibenzalacetone derived center were studied in which three of them presented mesomorphic behavior (**E-C12**, **E-3C12** and **EE-C10**). While the **O-C12** molecule did not show mesomorphism, indicating a minimum anisometry for DBA, the product **E-C12** exhibited a dark conglomerate mesophase between 171 and 140 °C. The increase of the number of peripheral long alkoxy chains initially suppressed mesomorphism (**E-2C12**), to later stabilize a Col$_h$ (**E-3C12**), as suggested by the texture observed by POM and XRD data. Finally, a new increase in molecular length promoted a polymorphism for **EE-C10**, which displays both a SmC and a B1 phase, the latter being characteristic for bent-shape liquid crystals. The results show that DBA is promising for the development of BCLCs, presenting mesophase variability and good thermal stability.

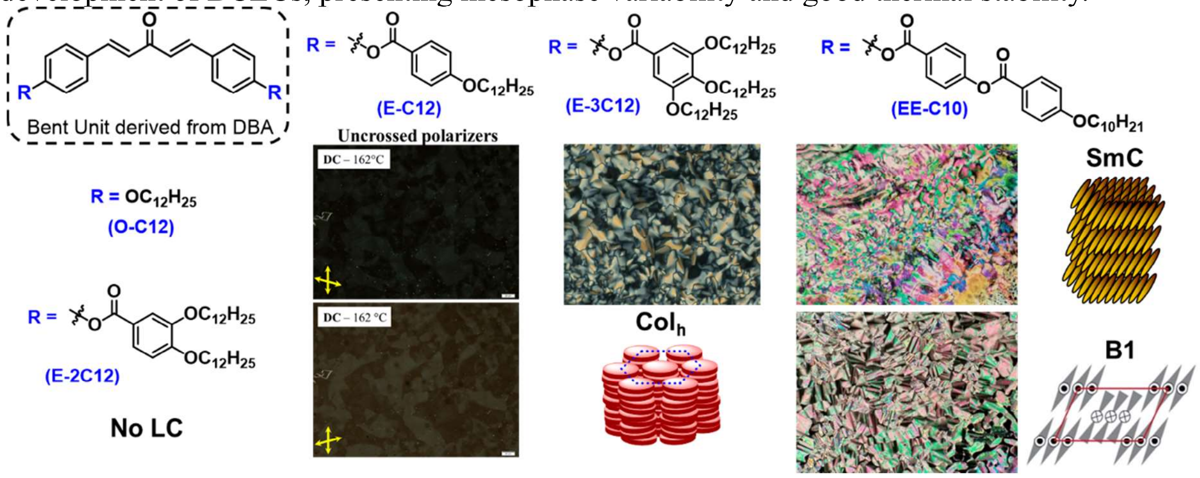

Figure 1: Curved structures derived from DBA synthesized in this work, together with observed and proposed mesophase textures.

Acknowledgements: UFSC, UTFPR, CNPQ, CAPES, INCT-INEO.

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Can solution studies offer insights into LC behavior?

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Keywords: columnar phases, conformation, discotic, dimers, NMR, DFT

Because molecular shape is a critical factor governing supramolecular organization in liquid crystals, material scientists typically rely on shape-persistent mesogens that organize in predictable, albeit limited, ways. In contrast, Nature routinely uses flexible building blocks to achieve an incredible range of complex biological nanostructures. In order to harness the considerable potential of flexible mesogens in LC design, our group has been investigating the relationship between bulk properties and the dynamic structures of molecules.

During routine characterization, we noted that discotic dimers composed dibenzophenazine groups connected by flexible linkers exhibited complex conformational dynamics in solution. Detailed NMR investigations indicated that these molecules adopt both compact (folded) and extended (unfolded) conformations; the degree of folding and the geometries of the individual conformers were found to strongly depend on the nature of the linking group. These structural changes were also accompanied by dramatic changes in mesophase stability, which prompted us to consider whether solution-phase dynamics, alongside DFT calculations, could provide insights into the thermotropic liquid crystal properties of flexible dimers.

In this presentation, I will provide an overview of our efforts to untangle the subtle interplay between molecular structure, conformation, and liquid crystallinity for a growing family of discotic dimers. These multi-pronged studies include synthesis, theoretical modelling and spectroscopic experiments aimed at uncovering the structural features that govern folding in solution and their implications for liquid crystal behavior. Although these relationships are often complex, our findings provide a new perspective on materials properties based on dynamic rather than static molecular structures.

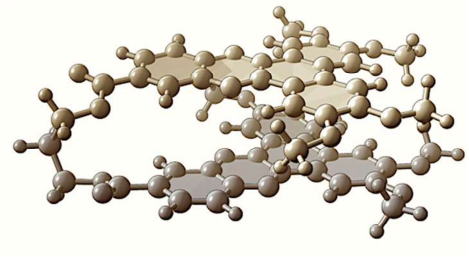

Figure 1: A folded discotic dimer

Acknowledgements: This work was funded by Natural Sciences and Engineering Research Council of Canada (NSERC).

Chiral Liquid Crystal Dimers: Synthesis, Mesomorphic Properties, and Helical Dynamics

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Keywords: LC dimers, Chirality, Spacer parity, Chiral hierarchy

Chiral liquid crystals (LCs) exhibit distinctive optical and mechanical properties, making them promising functional soft materials with potential applications in both scientific research and advanced technological applications.[1] The introduction of chirality into liquid crystals leads to the formation of helical structures, achievable by incorporating a stereogenic center within the LC molecule itself or by adding chiral mesogenic or non-mesogenic dopants into the LC host.[2] Chiral LC phases, characterized by increased complexity and unique properties, are the focus of our investigation.

Herein, we present the synthesis and mesomorphic properties of a series of LC dimers with a chiral centre as a part of their flexible spacer (Figure 1). Prepared dimers vary in spacer length and parity and were synthesized in both racemic and enantiomerically pure form. This allowed us to investigate the influence of spacer parity on mesomorphic behaviour and compare the LC phases generated by both racemic and chiral LC dimers.

By increasing the spacer length we affected the effective bending angle, resulting in the formation of both racemic and chiral forms of the twist bend nematic (N_{TB}) phase. The morphological differences between these two forms were significant, leading to the observation of hierarchical chiral structures in the N^*_{TB} phase. Furthermore, we investigated the ability of chiral dimers to induce helical organization in the nematic phase of different nematic hosts. An evident odd-even effect was observed in the helical twisting power (HTP) values. These results contributed to general understanding of how intrinsic chirality, located in the spacer of LC dimers, influences the overall structural chirality.

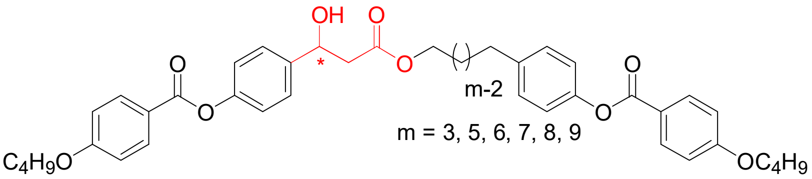

Figure 1: General structure of synthesized dimers.

Acknowledgements: The authors thank the Croatian Science Foundation [grant ref. IP-2019-04-7978 and DOK-2020-01] for financial support.

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Click for Light: Synthesis of Bent (Benzothiadiazolyl)triazole Luminescent Liquid Crystals via Click Chemistry

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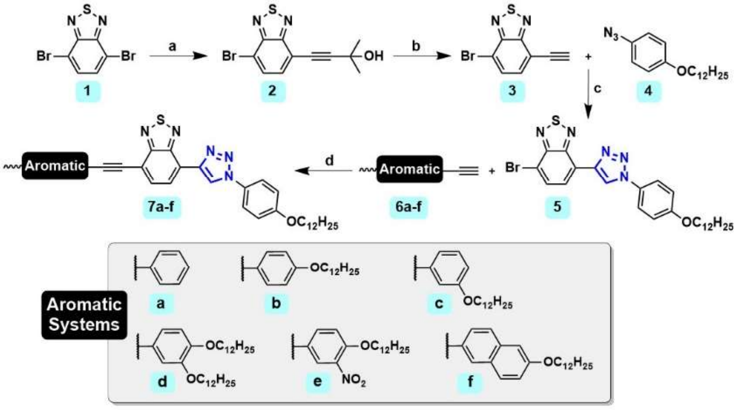
Keywords: 2,1,3-benzothiadiazole, triazole, luminescence, liquid crystals.

We report the synthesis and study of bent (2,1,3-benzothiadiazolyl)triazole (BTT) derivatives with different peripheral units connected to the BTT core via triple bonds. The click reaction was used as a tool to construct the central unit (benzothiadiazolyl)triazole. The molecules exhibited calamitic mesomorphism when long alkoxy groups terminally substituted them. These compounds combined smectic liquid-crystalline self-assembly with strong fluorescence not only in solution but also in the condensed state. The BTT derivatives show intense photoluminescence in the yellow region (510 to 555 nm) and with quantum yields that reach 90 % efficiency both in solution and in thin films. DFT calculations indicate dihedral angles of 29-31° between the benzothiadiazole and triazole rings, which may suppress pi-stacking and consequently reduce fluorescence quenching in the solid phase. They also show potential for specific detection of iron ions by selective fluorescence quenching. This work demonstrates that the (2,1,3-benzothiadiazolyl)triazole system is viable for preparing luminescent liquid crystals with high quantum efficiency.



Reagents and Conditions: (**a**) 2-Methylbut-3-yn-2-ol, $PdCl_2(PPh_3)_2$, CuI, PPh_3, NEt_3; (**b**) K_3PO_4, KOH, toluene; (**c**) CuI, NEt_3, $EtOH/H_2O$; (**d**) $PdCl_2(PPh_3)_2$, CuI, PPh_3, NEt_3/THF.

Figure 1: Synthesis of the target molecules 7a-f.

Acknowledgements: CAPES, CNPq, INCT/INEO, FAPESC, and FAPESB (PIBIC).

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Combination of rod and disc units as mesogenic molecules

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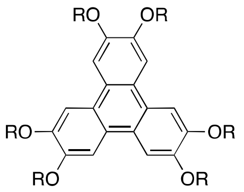
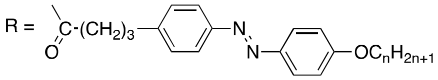
Keywords: liquid crystal, molecular conformation, calamitic mesogen, discotic mesogen

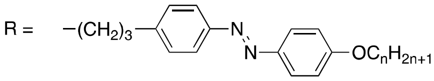
Rod and disc are two categories of mesogen in terms of anisotropic shape of molecules and the mesomorphic properties of combination of these parts (rod and disc) have been so far studied as mixtures. It was found that the combination of tetradecyloxyazobenzene as a rod part and a triphenylene as a disc part which are covalently bonded with an propylene-ester linkage exhibits SmA-Colr phase transition in both thermal and photonic processes [1] and recently the mechanism was studied to propose that the conformation change surely takes place at the SmA-Colr phase transition (Fig.1) [2]. For the dodecyl homologue, the ester and ether linkage derivatives were reported on their mesomorphism to give softness of the linkage significantly affect the variation of mesomorphism [3]. In this work, the comparison of mesomorphism of the ester and ether analogues (**1-Cn-3** and **2-Cn-3**, respectively) is shown to discuss on the relation of mesomorphism to the alkyl chain length as well as the linkage group.



1-Cn-3



2-Cn-3



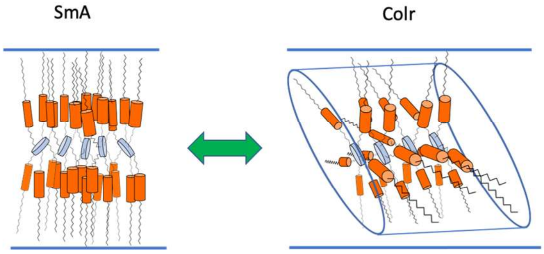


Fig.1 proposed mechanism of SmA-Colr phase transition (thermal).

In both alkyl homologues, some compounds exhibit calamitic-discotic mesophase transition. However, the richer diversity of mesophase was seen for the ether analogues (**2-Cn-3**) and the mesophase thermal stability is decreased in comparison to the ester ones (**1-Cn-3**), probably due to the flexibility of linkage part.

Acknowledgements: This work was supported by JSPS KAKENHI Grant Number 19K05630 and 15K05488.

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Design of new materials exhibiting polar & modulated liquid crystal phases

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Keywords: twist-bend phases, chirality, ferroelectric nematic phase, molecular design, structure-property relationships

The simplest liquid crystal phase – the nematic phase – is nowadays ubiquitous in our daily lives, and its ability to switch on application of an electric field underpins much of the multi-billion-pound liquid crystal display industry. Current LCD technology is limited by the speed at which the nematic phase can 'switch' and for this reason – and of course scientific curiosity – we seek new liquid crystal phases with the possibility of transformative applications in displays and beyond. Two such 'new' phases, for which recent studies appear to show incredible potential, are also nematic in nature – the twist-bend nematic phase, N_{TB},[1] and the ferroelectric nematic phase, N_F.[2] More recently, heliconical twist-bend smectic C (SmC_{TB}) phases have also been discovered for liquid crystal dimers[3] and it appears that a range of variants of this phase, similar to the SmC* subphases observed for chiral molecules, are possible.

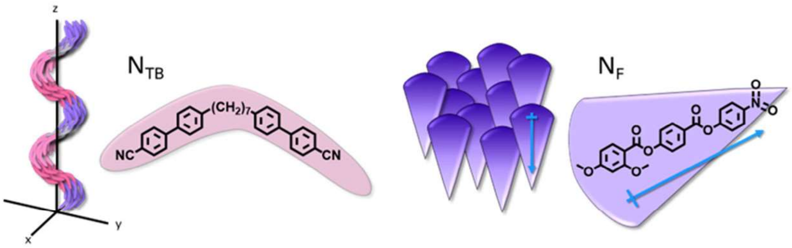

Figure 1: General structure and archetypical molecules of the N_{TB} (left) and N_F (right) phases.

From a chemist's perspective, understanding the molecular features influencing the formation and stabilisation of these new phases is of paramount importance, and allows for the design of new materials that have targeted properties. As such, recent work in Aberdeen has had the primary aim of enhancing our current understanding of these relationships in dimeric[4] and low-molar-mass liquid crystals,[5] through the synthesis and characterisation of a diverse range of materials.

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Dimers with chiral spacer – novel material with puzzling properties

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Keywords: LC dimers, Chiral spacer, Synthesis, Mesomorphic behaviorur, Chirality transfer

Liquid-crystalline dimers are intriguing materials due to their unique mesomorphism,[1] spontaneous chiral N_{TB} phase formation,[2] and their ability to stabilize specific properties important for technology when used in mixtures.[3] However, dimers with a chiral spacer are rare.

The synthesis and mesomorphic behavior of a novel series of dimers containing 3-aryl-3-hydroxypropanoic ester subunit (Fig. 1) will be presented. The chiral moiety containing the hydroxyl group at the stereogenic center was successfully incorporated into the spacer without losing liquid-crystalline properties in the bent-shaped dimers. These dimers were prepared in both racemic and enantiomerically pure forms, with different spacer lengths, parity, and aromatic mesogenic units. The discussion will focus on the impact of spacer chirality and parity, as well as the effect of different aromatic mesogenic units on chirality transfer from molecular to multiple levels of structural chirality.

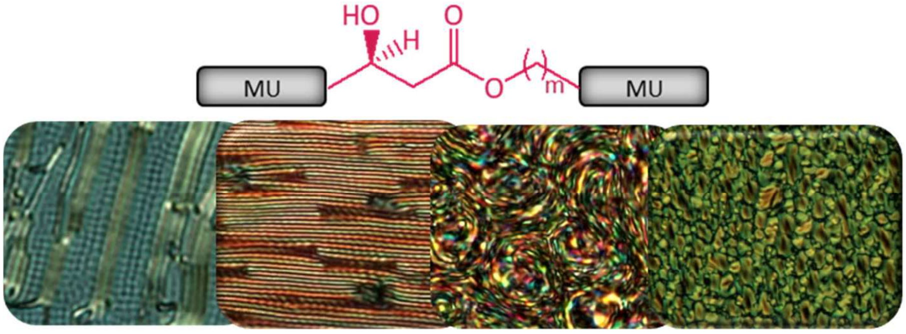

Figure 1: General structure of the chiral dimers and some of their unusual POM textures

Acknowledgements: The authors thank the Croatian Science Foundation [grant ref. IP-2019-04-7978 and DOK-2020-01] for financial support.

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Effect of Different Orientation of An Ester Group on Mesomorphic and Gelation Properties of Phenyl Benzoates Containing A Fluoroalkyl Chain

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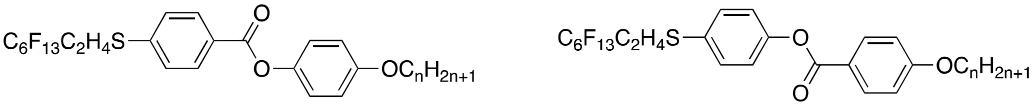
Keywords: Fluoroalkyl Chain, Phenyl Benzoate, Low Molecular Gelator, Structural Analysis.

It is well-known that some of rod-shaped phenyl benzoates containing a polar functional group behave thermotropic liquid crystal materials. In our previous study, it has been reported that some of 2-alkoxy-6-[4-(2-perfluorohexyl)ethylthiophenyl]naphthalenes exhibited a smectic A phase and gelatinized several organic solvents. [1] In this study, phenyl benzoates containing a fluoroalkyl chain (Figure 1) were synthesized and evaluated mesomorphic and gelation properties.



Compounds **1**-n (n = 1 – 12)

Compounds **2**-n (n = 1 – 12)

Figure 1: Chemical structures of compounds **1**-n and **2**-n.

Phase transition temperatures were analyzed using differential scanning calorimetry and a polarized optical microscope (POM). Compound **1**-8 an exothermal peak at 105 ºC (latent heat; $\Delta H = 38.6$ kJ mol^{-1}) on a heating process and detected two endothermal peaks at 97 ºC ($\Delta H = -27.1$ kJ mol^{-1}) and 103 ºC ($\Delta H = -10.0$ kJ mol^{-1}) on a cooling process. On the other hand, compound **2**-8 detected two exothermal peaks at 79 ºC ($\Delta H = 26.7$ kJ mol^{-1}) and 95 ºC ($\Delta H = 11.6$ kJ mol^{-1}) on a heating process. When each compound in bulk state observed using a polarized optical microscope, it formed a typical focal conic fan texture (Figure 2). Liquid crystal phases of compounds **1**-8 and **2**-8 can assign to be a monotropic and an enantiotropic SmA phases, respectively. In addition, compounds **1**-8 and **2**-8 which added in amount of 3wt% or less were able to gelatinize propylene carbonate.

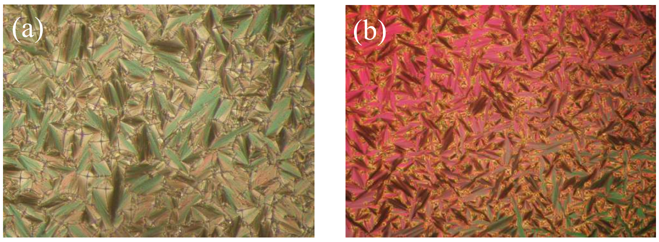


Figure 2: Images of polarized optical microscope observation for (a) **1**-8 (90 ºC on a cooling process), (b) **2**-8 (100 ºC on a cooling process).

In this presentation, effect of mesomorphic and gelation properties on elongation of a terminal alkyl chain and structural analyses of organogels using spectroscopic and computational studies will be also reported.

Acknowledgements: This work financially supported by JST SPRING [JPMJSP2111], JSPS KAKENHI [22H03781], and Paloma environmental technology development foundation.

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Electropolymerization Process applied to Liquid Crystalline Methacrylic Monomers

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Keywords: Polymers, Methacrylic monomers

This work focuses on the synthesis and characterization of a family of side chain liquid crystalline polymers of 4′-alkyloxyphenyl 4-(6-(methacryloyloxy)hexyloxy))benzoate. These polymers were obtained by an electroinduced polymerization [1] of their respective monomers [2]. All polymers shown enantiotropic mesophases. Shorter EP polymers shown nematic and SmA phases, while longer ones SmA and SmC phases, unlike their acrylic counterparts previously studied [3]. An interesting feature is the transition from single layer to double layer smectics phases when the terminal chain in the monomer increases from 4 to 5 methylenic units.

The phase diagram obtained is depicted in Fig 1 and was constructed by obtaining the transition temperatures by modulated differential scanning calorimetry (MDSC), while the mesophases identification were determined either by TD-XRD or wide-angle x-ray scattering (WAXS).

Polarized optical microscopy (POM) observations were also carried out during the polymerization process, and despite the alignment in the samples and the low mobility of the phases obtained it was useful for differentiating between nematic and smectic phases.

The new polymerization process is a powerful technique that can be synergistically employed in specific applications, especially in the development of advanced liquid crystal devices and optoelectronic systems.

Acknowledgements:

Fondecyt 1241746 and EQM200266 projects are gratefully acknowledged.

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Experimental and computational study of the effect of alkyl chains on thermal behavior of non-symmetrical Imidazophenanthroline (ImPhe)-based mesogens.

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Keywords: Soft materials, Imidazophenathroline, Thermal properties, Self-assembly, ImPhe.

The understanding of self-assembly features is crucial to the development of soft materials.[1] Imidazophenanthroline (ImPhe) is a promising *N*-heterocyclic nucleus for application in materials science, but it is still poorly explored in the field of liquid crystals.[2] This work reports an experimental/computational-combined study for the understanding of the thermal behavior of three non-conventional and non-symmetrical ImPhe-based mesogens (Fig. 1a). Our preliminary findings based on POM and DSC techniques show that the length of the alkyl chains affects considerably the thermal behavior. While the presence of two octyl chains in 1a does not induce mesophase formation, decyl and dodecyl chains, in 1b and 1c, respectively, result in monotropic and enantiotropic liquid crystals. Notably, compound 1b presented Smectic X (SmX) mesophase on cooling from 131 ºC to -20 ºC (Fig. 1b). On the other hand, compound 1c, on heating, presented SmX mesophase from 130 ºC to 24 ºC, and, and Glassy Smectic X (*G*SmX) mesophase on cooling (Fig. 1c). Computational results suggest that self-assembly of the dimers of each ImPhe derivative is strongly driven by π-π stacking interactions, which becomes less pronounced when longer alkyl chains are presented, such as in the comparison of compounds 1a and 1c (Fig. 1d), and this feature can be correlated to the variations in the observed thermal properties.

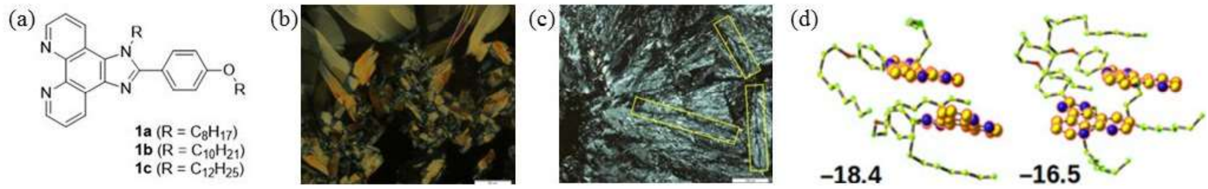

Figure 1: a) Chemical structures of ImPhe; b) Microphotograph of compound 1b in the SmX mesophase; c) Microphotograph of compound 1c on the *G*SmX mesophase; d) Lowest energy conformers of the dimers of 1a (left) and 1c (right) and their calculated energies (in kcal/mol).

Acknowledgements: CAPES, CNPq, Finep, FAPERN, Central of Analysis/IQ-UFRN.

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Gelation ability and self-assembly phenomena of liquid crystal materials having a coumarin skeleton at the terminal position

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Keywords: Synthesis, Molecular arrangements, Smectic phase, X-ray diffraction, Molecular gels, Thermal property

Generally, liquid crystal (LC) phases and molecular gels are known as one of the self-assemble phenomena of molecules, and of interest from the viewpoint of their molecular arrangements and structures. However, the correlation between the LC phase and the self-assembled structures of molecular gels is not clear.

Recently, we reported several LC materials having a coumarin skeleton show gelation ability in various organic solvents [1–3]. Here, we report that the physico-chemical property and the molecular arrangements in a smectic A phase for LC materials having a coumarin skeleton (Figure 1, compounds **1**-n and **2**-n).

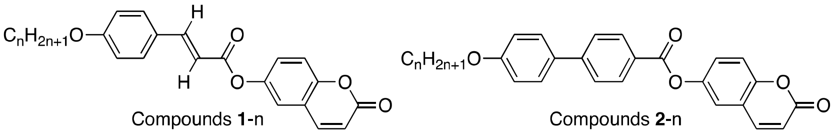

Figure 1: Molecular structures of compounds **1**-n and **2**-n

Table 1 shows phase transition temperatures in a bulk state under DSC measurement and polarity microscope observation. Compounds **1**-n and **2**-n exhibit an enantiotropic smectic A (SmA) phase and the thermal stability of the SmA phase increased on ascending the homologue. In addition, the homologs with an octyloxy group (n = 8) also exhibit an enantiotropic nematic phase. Interestingly, compounds **2**-n were able to form molecular gels with organic solvents such as 1-octanol and DMSO by added in an amount of 5% or less.

The molecular arrangements in the SmA phase and molecular gels will be discussed in terms of the molecular shape and electrostatic nature of the molecules.

Table 1: Transition temperatures for compounds **1**-n and **2**-n

Comp.	Transition temperature / °C *
1-6	C 131 I
1-8	C 126 SmA 130 N 135 I
1-10	C 119 SmA 138 I
1-12	C 113 SmA 145 I
2-6	C 149 N 240 I
2-8	C 151 SmA 208 N 232 I
2-10	C 125 SmA 205 I
2-12	C 110 SmA 225 I

*; C, SmA, N, and I indicate crystal, smectic A, nematic and isotropic phases, respectively.

Acknowledgements: This work financially supported by JSPS KAKENHI [22H03781], JST SPRING [JPMJSP2111], and Paloma environmental technology development foundation.

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Hidden architectures in the volume gap between triangular and square honeycomb liquid crystals

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Keywords: Bolapolyphiles, Liquid crystalline honeycombs, Tiling patterns

Complex modes of soft self-assembly can generate liquid crystals with interesting micro- and nanostructures. Such structures have been intensively studied for X- and T-shaped bolapolyphilic molecules having π-conjugated rods with sticky glycerol groups at both ends and one, two, or more side-chains.[1,2] These molecules form LC honeycombs and network structures. The honeycombs can be described by their projection on the plane as tiling patterns. Here, the transition between triangular and square tilings is of particular interest, because of the large area difference between them, new complex LC phase structures, including quasicrystalline LC and their approximants, can be expected to occur at the transition between them.[3,4] In a collaborative project between mathematics and chemistry, we searched for a general concept to optimize the search for these new LC structures. Considering the symmetry properties of the tilings and their transitions, and by abstraction of the main features of the molecular structure, the chemical details were reduced to geometrical problems. This enabled us to predict the molecular structural parameters required to achieve the envisaged LC tiling patterns. These predictions allowed the reduction of the chemical space to be explored, thus increasing the efficiency of materials synthesis as only a few compounds - with the highest probability to show the desired mesophases - have to be synthesized.[5] This approach is exemplified with molecules derived from a bolaamphiphilic oligo-(*p*-phenylene ethynylene) (OPE) core with two highly branched carbosilane side chains. Considering the predictions, the selected compounds were synthesized, and investigated by polarizing microscopy, DSC, and X-ray scattering. The observed tiling patterns were compared with the predictions and the gained insights were in a feed-back loop used to improve the mathematical model further.

Acknowledgements: This work was founded by the Deutsche Forschungsgesellschaft (DFG, 436494874 – RTG 2670).

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Liquid crystals based on thioether linkage: Difference in rod-like and bent molecules

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Keywords: (sulfur, thioether, birefringence, liquid crystal dimer, twist-bend nematic phase)

We present distinct effects of sulfur-based thioether linkage (C–S–C) on calamitic liquid crystals (LCs) with linear or bent molecular shapes. C–S–C is bulkier than classic $C–CH_2–C$ and C–O–C because of its more flexibility and smaller bond angle, as shown in Figure 1. Consequently, the thioether bond often disturbs LC formation for linear, rod-like molecules, thereby resulting in non-mesogenic, monotropic LC nature, narrow LC temperature ranges, and low phase traisition temperatures [1–4]. In addition, a more polarizable sulfur atom contributes to high reflractive index and birefringence of organic materials [2, 3]

In contrast, when the thioether bond is introduced at the linker position between a central spacer and mesogenic groups in bent LC dimers, greater bent shapes could be obtained compared to those achieved with their methylene- and ether-linked counterparts. This is remarkably advantageous for inducing LC phases, especially for a heliconical twist-bend nematic phase [5]. The effects of the thioether bond on inducing LC phases strongly vary depending on its positions and applied molecular shapes.

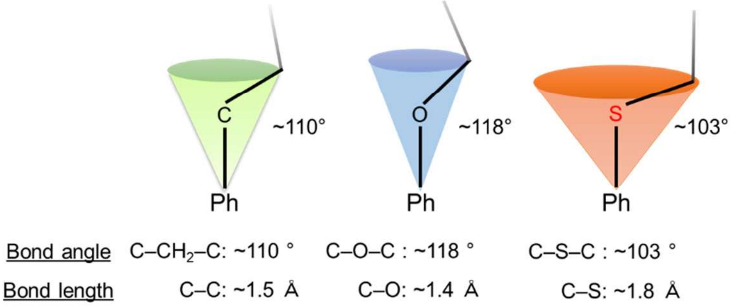

Figure 1: Basic bond characteristics of methylene, ether, and thioether linkages [4].

Acknowledgement

We are grateful for financial support JSPS KAKENHI (Grant Numbers 15H06285 and 17K14493).

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Low melting BTBT mesogens with ambipolar charge carrier transport

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Keywords: Smectic liquid crystals, BTBT, phthalocyanine, ambipolar charge carrier mobility

Star mesogens with conjugated arms and a phthalocyanine core **1** (Figure) self-assemble in a unique click process when mixed with a sterically crowded fullerene derivative [1]. The resulting nanoscale LC donor-acceptor structure is potentially of interest for photovoltaic applications.[2] Benzothienobenzothiophene (BTBT) compounds are excellent LC semiconductors that exhibit extraordinarily high charge carrier mobilities.[3] Therefore, it is attractive to replace the conjugated arms of stars **1a** or **1b** with a BTBT unit. A swallow-tailed siloxane moiety was chosen as the flexible periphery, which is known to strongly lower the clearing temperatures.[4]
This contribution describes the challenging synthesis of novel unsymmetric BTBT arms **2**-**4** with various functionalities (Figure 1). The phthalonitrile **2** has been prepared for a subsequent tetramerization yielding the corresponding phthalocyanine **1c**. While **1c** does not generate mesomorphism, the calamitic precursor **2** exhibits a low viscous broad enantiotropic SmA phase with a clearing point of 178 °C and high ambipolar charge carrier mobilities of up to 1.1 10^{-2} cm^2/Vs. These results prompted us to synthesise a family of BTBT materials with various aromatic substituents, with the goal to lower the transition temperatures. Here we highlight the results of their thermotropic properties studied by polarised optical microscopy, differential scanning calorimetry and X-ray scattering techniques and complemented by the study of their optical properties by UV-Vis absorption spectroscopy.

Figure. Structures of the zinc phthalocyanine derivatives **1a-c** and the BTBT mesogens **2-4**.

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Mesomorphic and Dielectric Properties of Strategically Designed Chiral Bent-Core Liquid Crystals Displaying Wide-Range Dark Conglomerate Phase

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Keywords: (Mirror Symmetry Breaking, Chiral conglomerates, DC phase)

In order to advance the scope of chiral functional materials, it is of paramount importance to engineer chiral bent-core liquid crystals (LCs) endowed with exceptional stability across a broad range of temperatures. In this context, we have devised a strategic approach, utilizing the potential of fluorinated molecules and taking advantage of the chirality of cholesterol as the pivotal component. This synergy has enabled the successful synthesis of our target LCs **nF-4R**. These molecules exhibit a chiral dark conglomerate (DC) phase over a broad temperature range of ~85 °C in an enantiotropic manner. Dielectric spectroscopy measurements conducted on these materials showed persistent dielectric behavior over the entire LC range. Our study stands as a pioneering exemplar, unveiling the long-range DC phase within the intricate landscape of chiral bent-shaped molecular systems. The mesomorphic characterization utilizing polarized optical microscopy, differential scanning calorimetry, and small-angle/wide-angle X-ray scattering measurements, revealed an optically isotropic DC phase. This phase shows domains of opposing chirality and belongs to the sponge-type DC phase. Notably, the enhancement of a specific chiral domain reveals the bias towards supramolecular chirality, attributable to molecular chirality as supported by circular dichroism measurements. This finding holds promise for chiral plasmonics, enantiomeric separation, and nano-templating applications.

Acknowledgements: IISER Mohali and CeNS for research facilities, SERB-TARE for funding, MoE Govt. of India for Prime Minister's Research Fellowship (PMRF)

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Mesomorphic and photophysical properties of new calamitic quinoxaline-based liquid crystals

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Keywords: Calamitic liquid crystals; Quinoxaline; Nematic; Smectic; Fluorescent; AIEE.

Liquid crystals (LCs) are relevant materials for academic and technological interest.[1] Quinoxaline is a heterocyclic nucleus highly explored in LC, however its use is practically restricted to discotic mesogens.[2] In this work, we present the liquid crystalline behavior and photochemical properties of four 4-(quinoxalin-2-yl)phenyl 4-alkoxybenzoate-based hockey-stick like mesogens (Fig. 1a). POM and DSC analysis showed that all quinoxaline derivatives were enantiotropic nematic and smectic LC (exemplified in Fig. 1b and Fig. 1c for compound QX1), with interesting mesophase ranges (up to 111 ºC on cooling). The photochemical behavior of the target compounds showed that presence of methyl groups in DMQX series induces considerably higher emissions, especially in methanolic solution (up to $\phi = 0.15$), and AIEE phenomenon was verified in acetonitrile solution, with emission up to 5.9 times higher ($\phi = 0.27$) when $f_w = 50\%$ (Fig. 1c). Photochemical results are supported by theoretical calculations. These results are very promising and with great interest to the development of calamitic fluorescent liquid crystals.

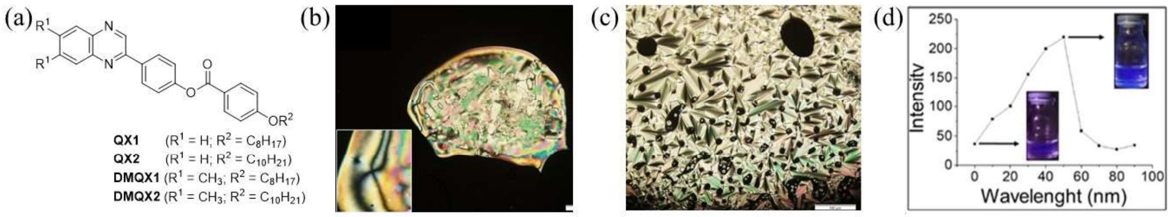

Figure 1: (a) Chemical structures of QX1, QX2, DMQX1 and DMQX2; (b) QX2 on cooling at 140 ºC entering in the nematic mesophase; (c) QX2 on cooling at 132 ºC in the SmA mesophase; (d) Emission *vs* f_w plot and photographs of solution of DMQX1 in acetonitrile solutions.

Acknowledgements: CAPES, CNPq, Finep, FAPERN, Central of Analysis/IQ-UFRN.

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New Semiconducting Mesogens by combining Subphthalocyanine Cores with Benzothienobenzothiophene Arms

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Keywords: Polar columnar liquid crystals, BTBT, subphthalocyanine

Subphthalocyanine star mesogens were recently reported to form highly polar lyotropic and thermotropic liquid crystals phases. [1] The subphthalocyanine core is of great interest as non-fullerene acceptor for photovoltaic applications. The bulk photovoltaic effect has been observed in well aligned samples [2,3], which turns these structures into attractive targets for materials science. Therefore, we coupled oligothiophene arms to the subphthalocyanine resulting in an umbrella-shaped mesogen (**1**)generating polar columnar dimer phases.[4] In the search for novel materials for organic electronics, the combination of the subphthalocyanine with benzothienobenzothiophene (BTBT) arms is an attractive target, as BTBT frameworks are among the best semiconductors known to date.[5]

Herein we present the challenging, successful synthesis of non-symmetric BTBT derivatives tailored for cross-coupling with the triiodosubphthalocyanine core via different linking units, resulting in target mesogens **2-4**. The impact of these units on thermotropic properties and the mesophase structure is studied by polarised optical microscopy, differential scanning calorimetry and X-ray scattering.

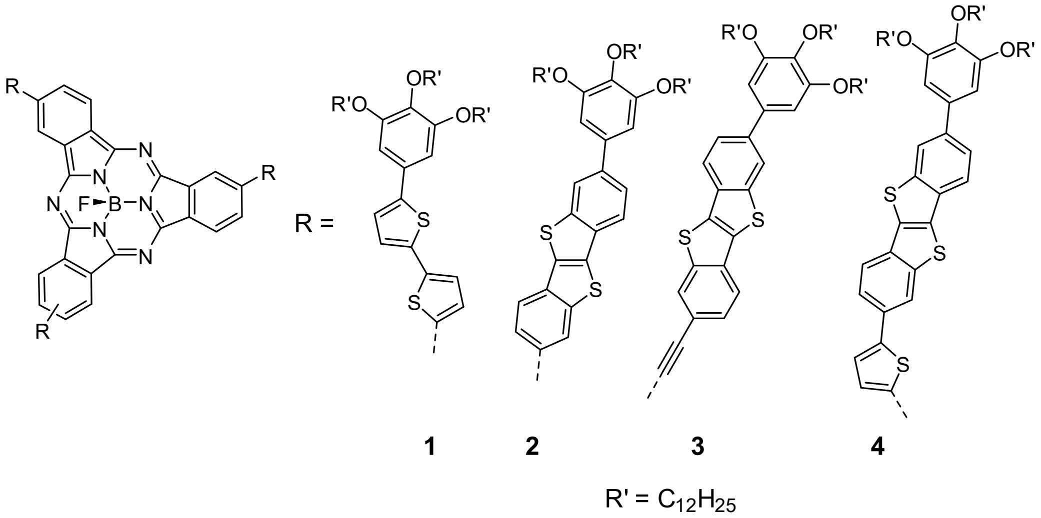

Figure. Structure of three different BTBT-subphthalocyanine star mesogenes.

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New tiling modes in LC honeycombs of rod-like bolapolyphiles combining fluorinated and non-fluorinated side-chains

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Keywords: Honeycomb liquid crystals, semi-fluorinated chains, nano-segregation

As shown in previous work, T-shaped and X-shaped polyphilic molecules provide a route to LC materials with new phase structures, such as honeycomb LCs and new types of network phases [1]. Here we report a series of oligo-(*p*-phenylene ethynylene) (OPE) based X-shaped molecules combining semi-fluorinated and non-fluorinated alkyl chains at opposite sides (Fig. 1). The compounds have been synthesized, and investigated by XRD and optical investigations, and the effects of temperature, side-chain length and core fluorination were studied. The volume of the lateral chains was chosen to be too large for triangular and too small for square cells, and their length was slightly modified. These compounds form multicolor tiling where prismatic cells containing the hydrocarbon chains and others containing the fluorinated chains form 2D superlattices derived from the square chessboard tiling [2] by cell shrinkage. One mode of shrinkage leads to a *p*4*gm* lattice composed of square and rhombic cells (angular deformation). A second mode of cell shrinkage takes place by tilting the molecules forming the walls, thus retaining the chessboard tiling with a smaller size ($p4mm^{T}$) and inverted sign of birefringence. Finally, cell deformation by tilting the molecules in only two opposite sides, while two sides remain non-tilted, leads to a chessboard-like tiling with rectangular cells (*c*2*mm*).

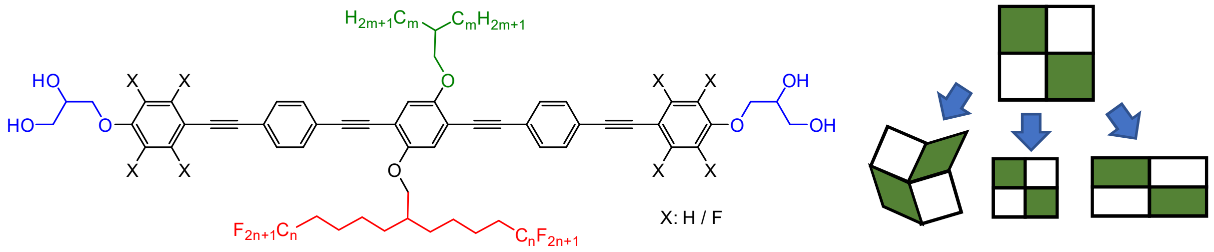

Figure 1: Molecular structure of the reported OPE-based bolapolyphiles and represntative two-color tiling patterns of the LC phases formed by these compounds.

Acknowledgements: This work was supported by the Deutsche Forschungsgemeinschaft (DFG, 436494874 – RTG 2670).

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Non-symmetric tristriazolotriazines with room temperature mesomorphism

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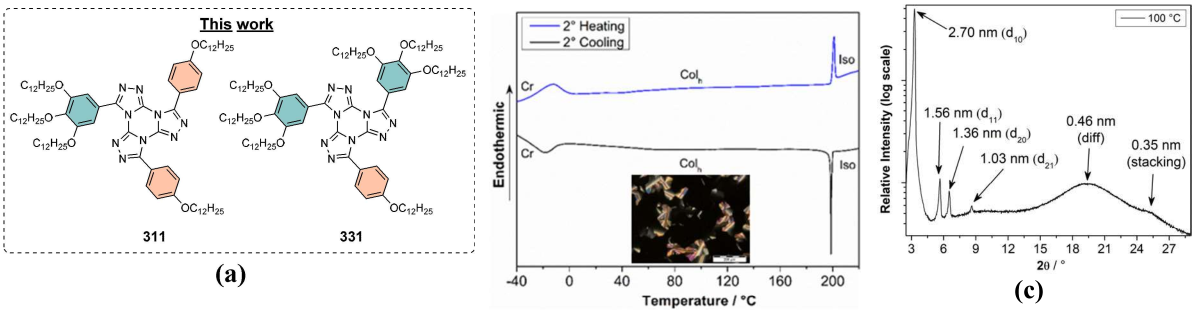
Keywords: Tristriazolotriazines, non-symmetry, columnar hexagonal, luminescence.

Molecular non-symmetry is a feature of interest in the liquid crystals (LCs) research due to the observed decrease in the transition temperatures, enhanced mesophase stability, and the prevention of crystallization through glass transitions, when compared to the symmetric compounds.[1,2] This behaviour is of great interest for technological applications. However, for the tristriazolotriazines (TTTs) based LCs research, to date, there has been no description of non-symmetric molecules, *i.e.*, those with unequal arms. Therefore, this work aims to fill this gap by reporting two non-symmetric compounds derived from the TTT core (**311** and **331**) (Fig. 1a). The non-symmetric **311**, presented a waxy appearance at room temperature, no mesomorphic behavior was identified, as well as no crystallization during the cooling processes, remaining in super cooled amorphous state. On the other hand, **331** presented room temperature Col_h phase with impressive stability, ranging from -13 to 201 °C (Figure 1b), significantly better than the 9-chain symmetric TTT, which presented Col_h between 133 and 177 °C.[3] The Col_h mesophase was confirmed by XRD, which showed a typical diffraction pattern in addition to the π-stacking broad peak (Figure 1c). Compound **311** and **331** presented intense fluorescence in the blue region with quantum yields of 52 and 35% in solution (37 and 67% in thin film), respectively, higher than the 6% reported for the 9-chain symmetric TTT. The findings show that non-symmetry is promising for the TTT derivatives, this being the first case reported, and whose behaviour may favour future applications attempts.



(a) (b) (c)

Figure 1. (a) Structures of the synthesized and investigated non-symmetric TTTs **311** and **331**. (b) DSC thermogram of **331** showing the wide range mesomorphism, in addition to the typical Col_h texture at 150 °C (crossed polarizers). (c) XRD pattern of the **331** Col_h mesophase at 100 °C.

Acknowledgements: UFSC, UTFPR, CNPQ, CAPES, INEO, UBx, CNRS/CRPP.

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Non-symmetric twisted core for discotic liquid crystals with delayed fluorescence and persistent room temperature phosphorescence

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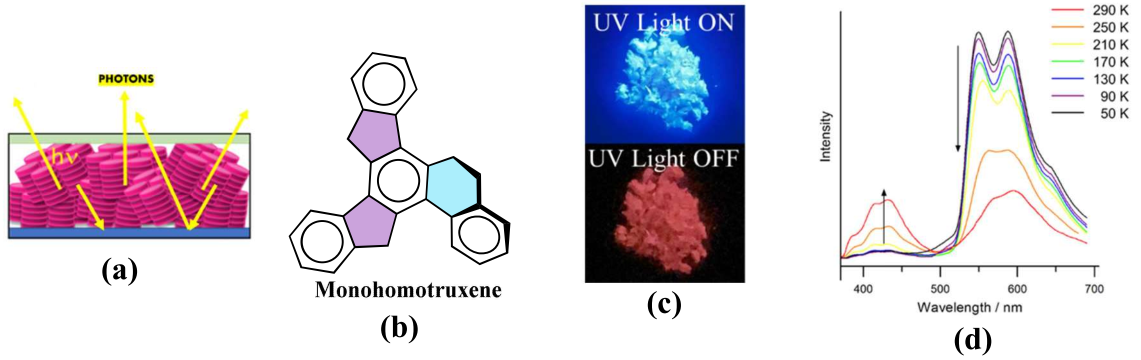
Keywords: Discotic LCs, delayed fluorescence, room temperature phosphorescence, twisted arenes.

The combination of liquid-crystalline and luminescent properties within a single compound is of great interest in organic optoelectronics, because it may yield anisotropically aligned light emitting materials.[1] The orientation of the mesogen dipoles relative to the device surface plays a fundamental role in mitigating photon losses attributed to inefficient light outcoupling (Figure 1a).[2] If the aligned emitter presents delayed luminescence, the electroluminescence can be enhanced.[3] Among pure luminescent organic molecules, homotruxene, i.e. sym-triphenyltriazine where three ethylene bridges lock the arene system into a triply twisted configuration, has shown delayed emission, but its twisted structure impedes liquid-crystalline behavior. To improve planarity without affecting photophysics, the non-symmetric "monohomotruxene" with one ethylene and two methylene bridges (Figure 1b) was designed, synthesized and characterized to assess it as a core for delayed-luminescent discotic liquid crystals. The molecule shows phosphorescence at room temperature (RTP) (Figure 1c and 1d), and delayed fluorescence (DF) by triplet-triplet annihilation (TTA). To combine such delayed emission with liquid-crystalline behavior, monohomotruxene is functionalized with multiple peripheral alkoxy substituents.



(a) (b) (c) (d)

Figure 1: (a) Anisotropic emission in an aligned OLED device by discotic mesogens; (b) off-planar monohomotruxene, (c) persistent orange phosphorescence observed when switching off the UV light, (d) delayed emission as a function of temperature in a condensed film.

Acknowledgements: This work is funded by the Franco-Brazilian cooperation CAPES-COFECUB 937-20 / Ph-C 962-20, and by CNPq.

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Oxadiazole-functionalized pyrene derivatives: Effects of alkyl-1,3,4-oxadiazole substituents on photophysical, electrochemical, and liquid crystalline properties

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Keywords: Pyrene; 1,3,4-Oxadiazole; Discotic Liquid Crystal.

Multifunctional materials are widely used in optoelectronic devices. 1,3,4-oxadiazole and pyrene core have such as good chemical and thermal stability and high fluorescence.[1,2] Furthermore, 1,3,4-oxadiazole has electron-accepting properties, while pyrene is a π-electron-rich group with rigid nucleus [3] with great potential for columnar liquid crystals.
Combining the properties mentioned above in the same material results in a good candidate for use in OLED devices. In this work, the synthesis of three new alkyl oxadiazoles from pyrene 1,3,6,8-tetracarboxylic acid [4,5] and the effects of alkyl-1,3,4-oxadiazole substituents on photophysical, electrochemical, and mesomorphic behavior were investigated, in order to obtain a discotic liquid crystal with high fluorescence to use in the construction of OLEDs. It was found that the 1,3,4-oxadiazole heterocycle is an excellent polar group for inducing columnar packing and, in addition, resulting in emitters with strong luminescence and promising for use in optoelectronic devices.

Acknowledgements: M.F. greatly acknowledges support from the Polish National Science Centre funding, grant no.: 2021/43/D/ST4/03017. We kindly acknowledge the support received under the CAPES-COFECUB program. The authors are also grateful to the CEBIME-UFSC, for the HRMS analysis, and LDRX-UFSC, for the XRD experiments.

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Photochemistry, AIEE and acidchromism of nonconventional 2,4,6-triarylpyridines

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Keywords: TAP; Photochemical; AIEE; acidchromism.

N-heterocycles are widely employed in the development of soft-materials due to their notable thermal, electrochemical and optical properties.[1] As an advance in the search for nonconventional structure-designed soft material, this work reports the photochemical behavior and acidchromism of new 2,4,6-triarylpyridine derivatives (Fig. 1a). The photochemical analysis shows that most emissive material in dichloromethane solution is the carbazole-derivative 1a (λ_{EM} = 406 nm; ϕ_f = 0.36), and a change in solvent (acetone) does not affect considerably the optical properties. Compound 1a is also the most fluorescent material in solid state. The effect of addition of water to the TAP derivatives in acetone solution indicated emission improvement when electron-releasing substituents (notably, carbazole) are present in the structure (Fig. 1b). The effect of the presence of acid in the aqueous acetone solutions of 1a and 1f (fluor-derivative) was investigated, and this later showed considerably more prominent acidchromism in f_w = 30%. This phenomenon was characterized by decreasing in the band at 388 nm concomitantly to an emerging band at 476 nm (Fig. 1c), and this results is in agreement to naked eye analysis. In addition, 1f-adsorbed paper strip was found to be very effective chemosensor for the detection of gaseous HCl by direct naked-eye analysis (Fig. 1d). Thermal properties of these TAP derivatives were investigated by POM and DSC, however, these nonconventional structure did not showed liquid crystalline behavior.

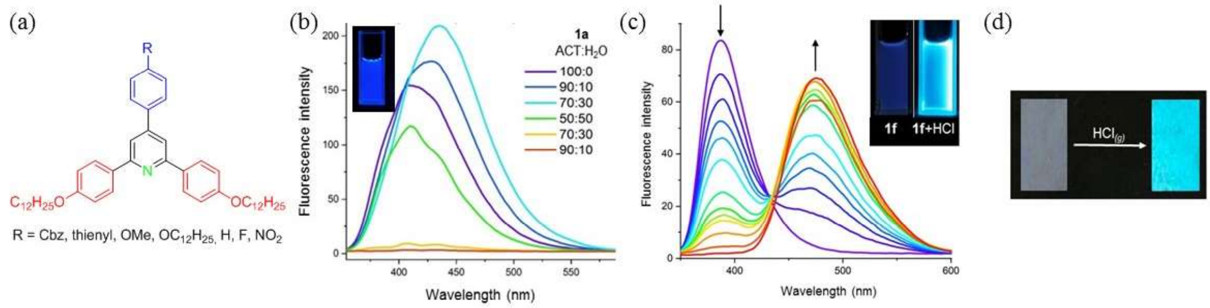

Figure 1: a) chemical structures of TAP derivatives; b) Fluroescence spectra of **1a** (1.0 µM) in aqueous acetone – insert: photograph of acetone solution; c) Fluorimetric titration of **1f** (100 µM) in aqueous acetone upon addition of HCl (pH 2.44 to 0.50) – insert: photophraphs of soluitons in pH 3.0 and 0.50); d) **1f**-adsorbed paper strips before and after interaction with gaseous HCl.

Acknowledgements: CAPES, CNPq, Finep, FAPERN, Central of Analysis/IQ-UFRN.

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Photophysical and structural features of mono- and di-octyloxystyrylquinoxalin-2(1*H*)-one derivatives

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Keywords: Styrylquinoxaline, photochemistry, *cis-trans* isomerism

Fluorescent small organic molecules are key to the development of many technological materials.[1] 3-Styryl-1*H*-quinoxaline-2-one (SQX) is a privileged scaffold due to the broad range application of their derivatives, including application in materials science.[2] In this work, photochemical and structural behavior of two SQX derivatives (Fig. 1a) is presented. Although the presence of one or two ocytloxy chains in SQX1 and SQX2, respectively, as well as the nature of the solvent (hexane, dichloromethane, acetonitrile, methanol) do not lead to representative differences in the UV-Vis data, these factors affect considerably their emissive properties (Fig. 1b). In general, higher wavelength emissions were verified in methanol (486 nm and 540 nm for SQX1 and SQX2, respectively). On the other hand, dichloromethane solutions presented higher intensity emissions. In addition, Stokes shifts for SQX2 are considerably larger than SQX1. It was confirmed the existence of reversible *trans-cis* isomerism for these SQX in the presence of UV-Vis light, and this phenomena affects UV-vis spectra of both compounds, but only emissive ability of SQX2. Computational results showed two thermodynamically comparable *trans*-isomers coexisting additionally to a less stable *cis* isomer. The addition of water to the methanolic solutions of SQX1 and SQX2 lead to higher emission up to f_w = 70% and 50% for SQX1 and SQX2, respectively. POM analysis and computational data suggest that the presence of one alkoxy chain leads to a lamellar H-bonding supramolecular organization whereas two alkoxy chains induces to a discotic H-bonding dimerization (Fig. 1c), however, none of these compounds were found to present liquid crystalline behavior. The structural and photophysical results reported in this work are of interesting to the development of fluorescent SQX-based materials and further applications.

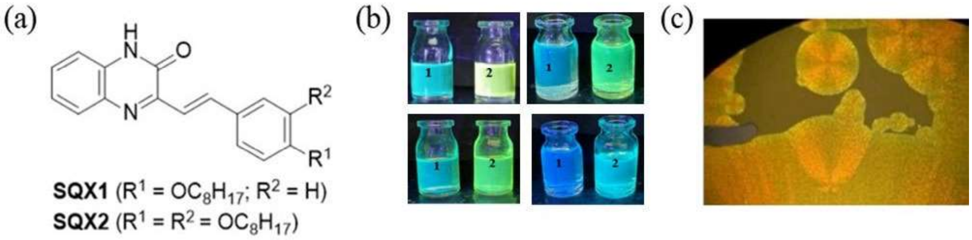

Figure 1: (a) Chemical structures of SQX1 and SQX2; (b) photographs of SQX1 (1) and SQX2 (2) in different solvents under light (365 nm) - clockwise: methanol, acetonitrile, dichloromethane, and hexane; (c) Microphotography obtained by POM for compounds SQX2.

Acknowledgements: CAPES, CNPq, Finep, FAPERN, Central of Analysis/IQ-UFRN.

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Probing linear dichroism and its optical orientation in perylene-derivative thin films via rotating-sample transmission spectropolarimetry

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Keywords: Spectropolarimetry, Anisotropy; Perylene; Langmuir-Shaeffer; Physical Vapor Deposition

Linear dichroism (LD) is a fundamental form of optical anisotropy arisen from light transmission through an anisotropic medium, and it is defined as the differential absorption of orthogonal linear states of incident light's polarization. Its measurement is commonly made by a direct acquisition of absorption spectra probing the sample with either two orthogonal incident polarization state, or with sample positioned at two orthogonal orientations (parallel and perpendicular to a fixed incident linear state). However, such procedures lack the benefits of a complete characterization of transmitted light, which contains full information about sample's anisotropies, and they are susceptible to a misplacing of the true optical orientation of the sample, since the required light-sample parallelism is roughly estimated. In this study, we develop an approach to acquire linear dichroism (LD) and its optical orientation data from the Stokes parameters of light transmitted by a rotating sample. The samples, carefully aligned in a rotating mount, are subjected to broadband vertically polarized light, and the transmitted light is analyzed using a rotating-retarder type of spectropolarimeter. By systematically varying the angular position of the sample, we obtain a complete set of Stokes vectors for each transmitted wavelength as a function of the angular position of the sample. The resulting modulation of Stokes parameters over sample orientation provide enough information for obtaining LD spectra and its optical orientation, i.e., the spectral difference between maximum and minimum absorption, and wavelength-dependence of the lowest-transmission axis direction. In order to illustrate that, we performed a set of measurements with organic thin film samples of a perylene-derivative; namely, bis-phenethylimide perylene-3,4,9,10-tetracarboxylic diimide (PhPTCD). Specifically, to corroborate meaningful anisotropy data, we performed two simple correlation studies. First, we compare the results for films produced by two deposition methods: Langmuir-Shaeffer (LS) and physical vapor deposition (PVD). Then, we display the results for two LS-PhPTCD films submitted to different thermal treatments; one kept at ambient conditions, and the other annealed at 200°C for 2h. Such analyses yield that LS films are anisotropic, showing significant LD signal, while PVD films are essentially isotropic, and that thermal treatment enhances LS-PhPTCD film's anisotropy. Our results agree with the presumed underlying mechanisms of each film deposition method and establish a prospect line of research in controlling and assessing the anisotropy of organic thin films, which can be deliberately engineered during sample fabrication.

Red NIR-Emissive Crown Ether Based Clustomesogens

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Keywords: Metal clusters, hybrid material, luminescence, charge transport

Creating organic-inorganic hybrids is still a promising way to improve processability or even trigger synergetic effects.[1,2] We present hybrids of discotic liquid crystals (DLCs) based on alkoxy substituted dibenzo crown ethers (CE) and near infra-red emissive molybdenum cluster compounds obtained via complexation. All hybrids showed a columnar hexagonal mesophase with a broader temperature range than the pure DLCs. Their lattice parameters derived from X-ray diffraction (XRD) analysis suggest a tighter packing for most hybrids. Changing the cluster's inner ligands from Cl^- to Br^-, showed an additional increase in temperature stability, as verified via differential scanning calorimetry (DSC) and polarized optical microscopy (POM). Emission properties vary depending on the inner ligand. For Cl^-, the average lifetime decreased for all clustomesogens in comparison to the pristine cluster. Their emission intensities diminish with rising temperature. The brominated cluster hybrids showed longer lifetimes and more stable emission intensities upon heating. In general, an increase in temperature lead to a slight blue shift of the emission maximum for all clustomesogens. Electrical conductivity could be increased at higher temperatures for all hybrids mostly depending on the chosen alignment method. Complexation of the molybdenum clusters led to improved electrical conduction in the liquid crystalline phase and therefore to an enhanced electronic transport within the CE.

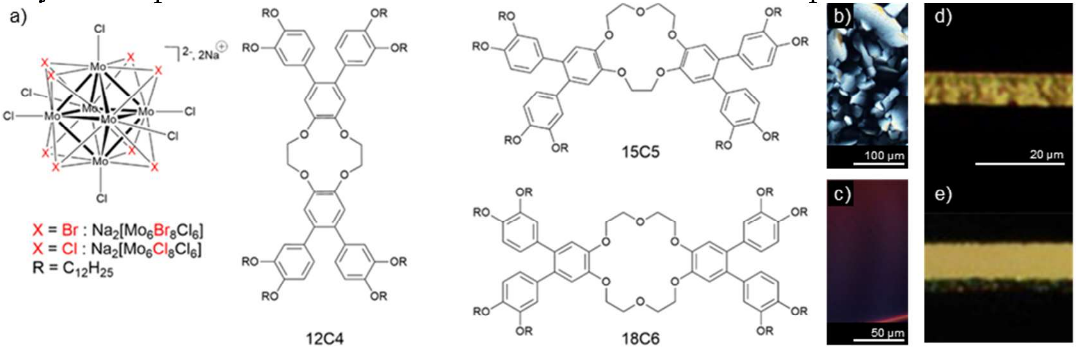

Figure 1: a) Schematic representation of the hybrids, textures of 15C5 • $Na_2[Mo_6Cl_8Cl_6]$ at b) 162 °C with white light and c) 180 °C with UV irradiation and photographs under polarized optical light for 18C6 • $Na_2[Mo_6Cl_8Cl_6]$ d) before and e) after electrical alignment.

Acknowledgements: Deutsche Forschungsgemeinschaft (LA 907/20-1), ANR „SNAPSTER“ (ANR-18-BS07-0003-01), PHC DAAD Procope project „PLISE“ #37689XA.

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Shining Future with New Near Infrared Emissive Ionic Liquid Crystal Clustomesogens

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Keywords: ionic liquid crystals, cluster compounds, organic-inorganic hybrid composites luminescence

Energy conversion for lighting and optoelectronics are current challenges. In order to find alternatives for rare earth oxides which are used for these applications, new luminescent hybrid materials have been developed by combining inorganic metal nanocluster $A_n[M_6Q^i_8X^a_6]$ (A = alkali, Q = chalcogen/halogen, X = halogen, M = Mo, Re) with organic ionic liquid crystals (ILCs). The inorganic moiety provides useful functionalities such as strong luminescence in the red near-infrared (NIR) region and robustness, while the organic counterpart (ILC) controls the long-range orientational order, the self-healing of defects and allows the material to be processed in common organic solvents.[1-3] We report here the first examples of red-NIR emissive ILC clustomesogenes made of phosphorescent octahedral molybdenum cluster anions associated with wedge-shaped cationic amphiphilic guanidinium minidendrons via ionic self-assembly (Figure 1).[4] Our results show that the mesomorphic properties are strongly affected by the complexation of amphiphilic guanidinium chlorides with metal clusters. Moreover, the length of the minidendron alkyl chain play a critical role regarding the luminescence of the metal cluster core.

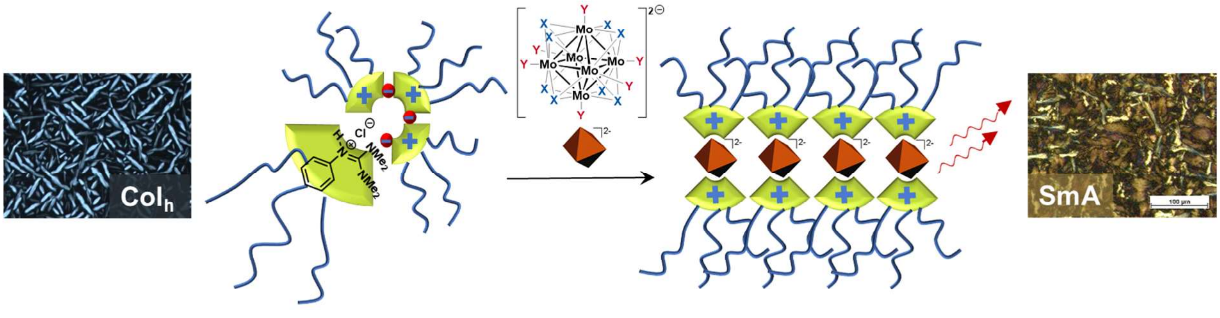

Figure 1: Emissive clustomesogens obtained by electrostatic association of octahedral cluster anions with amphiphilic minidendron cations. The Figure was taken and adapted from ref[4].

Acknowledgements: This work was funded by DFG-ANR (SNAPSTER) and DAAD-Procope (PLISE).

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Supertwisted Chiral Gyroid and Related Mesophases in Chiral and Achiral Polycatenar Compounds

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Keywords: chirality, gyroid, bicontinuous phases, polycatenars

Among the intriguing bicontinuous self-assembled structures, the gyroid cubic is the most ubiquitous. It is found in block and star polymers, surfactants with or without solvent, in thermotropic liquid crystals with end- or side-chains, and in biosystems providing structural color and modelling cell mitosis. It contains two interpenetrating networks of opposite chirality and is thus achiral if, as usual, the content of the two nets is the same (Figure 1a). However we now find that strongly chiral compounds can also form the gyroid cubic structure, but a chiral one instead. While achiral molecules follow the opposite twists of nets 1 and 2 in the gyroid structure, molecules with a chiral center in their rod-like core do not follow the 70° twist between junctions in net 2 and instead wind against it by -110° to still match the junction orientation. The metastable chiral gyroid is a high-entropy high-heat-capacity mesophase. The homochirality of its nets makes its CD signal close to that of the stable I23 phase with 3 isochiral nets. The relationship of this supertwisted chiral gyroid mesophase to other bicontinuous mesophases, in both chiral and achiral compounds, will be discussed too.

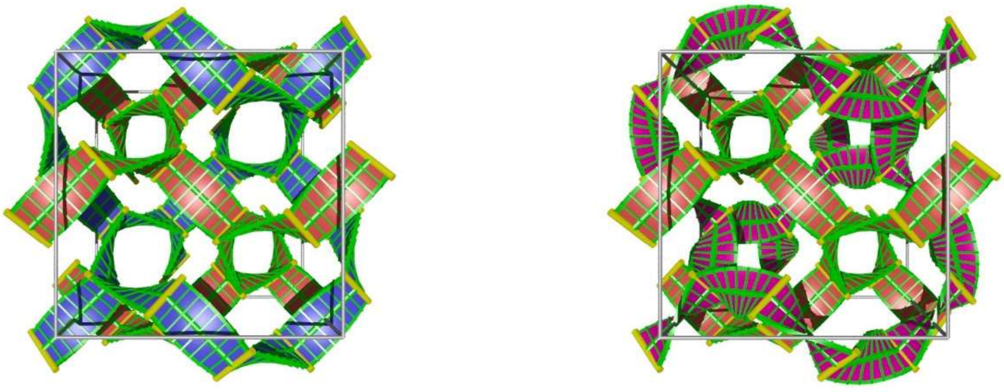
(a) (b)

Figure 1: Models of a gyroid unit cell using spine-and-ribs ribbons, each rib representing a raft with molecules parallel to rib. (a) Achiral and (b) chiral gyroid. The “supertwisted” net in (b) is shown in purple.

Syntheses, Mesomorphic and Gelation Properties of Phenyl Benzoates Core Containing Fluoroalkyl Chains

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Keywords: Synthesis, Fluorine, Phenyl Benzoate, Low Molecular-weight Gelator.

It is well-known that some of rod-shaped phenyl benzoates containing a polar functional group behave thermotropic liquid crystal materials. In our previous study, it has been reported that some of 4-semi-fluoroalkyl-4'-alkoxybiphenyls exhibited a smectic A phase and gelatinized several organic solvents. [1] In this study, phenyl benzoates containing fluoroalkyl chains (Figure 1) were synthesized and evaluated mesomorphic and gelation properties.

R = $-OC_8H_{17}$: Compound **1**-H
R = $-SC_2H_4C_6F_{13}$: Compound **1**-F

R = $-OC_8H_{17}$: Compound **2**-H
R = $-SC_2H_4C_6F_{13}$: Compound **2**-F

Figure 1: Chemical structures of compounds **1** and **2**.

Phase transition temperatures and critical gel concentrations of compounds **1**-H, **1**-F, **2**-H, and **2**-F are shown in Table 1. Compound **1**-F was non-mesogenic due to a high melting point, however, the others exhibited a smectic A phase. In addition, these were able to gelatinize propylene carbonate (PC) in adding less than 5wt% of the compound. As noteworthy points, compounds **2**-H and **2**-F were able to gelatinize PC with less than 1wt% addition since PC may interact with π electron by donor–acceptor interaction [2]. On the other hand, compound **1**-H were not able to gelatinize *n*-octane whereas the others were able to gelatinize. Self-assembly phenomena for gelation with compound **1**-H may not be interacted between terminal alkyl chains, resulting in solvation with *n*-octane.

Table 1: Phase transition temperatures in bulk state and critical gel concentrations.

Compounds	Phase transition temperatures / ºC a)	Critical gel concentration (wt%) b)
1-H	Cryst 79 SmA 95 Iso	*n*-Octane (Sol), PC (3.0)
1-F	Cryst 134 Iso	*n*-Octane (4.0), PC (4.0)
2-H	Cryst 86 SmC 122 SmA 131 Iso c)	*n*-Octane (4.0), PC (0.3)
2-F	Cryst 124 (SmA 113) Iso	*n*-Octane (2.0), PC (0.9)

a) Cryst, SmC, SmA, and Iso indicate crystal, smectic C, smectic A, and isotropic liquid phases, respectively. Parentheses indicate a monotropic transition. b) PC indicates propylene carbonate. Sol indicates sol state (i.e., it cannot be gelatinized, however, can be dissolved) with 5wt% addition. c) Cited from reference [3].

In this presentation, thermodynamic behaviors of gelation compared with phase transition in bulk state and rheological properties of organogels will be also reported.

Acknowledgements: This work financially supported by JST SPRING [JPMJSP2111], JSPS KAKENHI [22H03781], and Paloma environmental technology development foundation.

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Synthesis and Mesomorphic properties of cyclotriphosphazene compounds having fluoroalkylated mesogenic cores

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Keywords: Synthesis, Cyclotriphosphazene, Fluoroalkyl chain, Smectic phase, Organic gel, Perfluorotributylamine

Some organocyclotriphosphazenes with mesogenic side groups have been synthesized and the mesomorphic property are also investigated [1], however, the relationship between mesomorphic property and molecular arrangement are not clear. On the other hand, we have been reported that some liquid crystal materials having fluoroalkylated mesogenic cores exhibit smectic phases and form organic gels [2].

This paper describes synthesis and physico-chemical properties of cyclotriphosphazene derivatives having 4-perfluoroalkylethylthiophenyl group (compounds **1**-n and **2**-n).

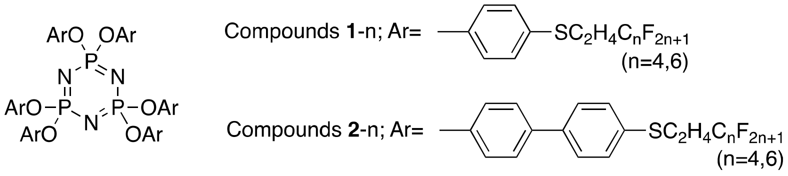

Figure 1: Molecular structures of compounds **1**-n and **2**-n.

Compound **1**-n and **2**-n were prepared by the nucleophilic substitution reaction of hexachlorocyclotriphosphazene. Their mesomorphic properties, which are summarized in Table 1, were examined by DSC measurement and polarity microscope observation. These compounds exhibited a smectic A (SmA) phase with a focal conic fan texture. The thermal properties of the SmA phase are examined using binary phase diagrams of the mixture of the compound **1**-6 and liquid crystal materials with a perfluoroalkyl group. These results will be discussed in terms of the relationship of molecular structures and the physico-chemical properties. In addition, compound **1**-6 was able to form organic gels in fluorous solvents such as a perfluorotributylamine, so these gelation properties will also be reported.

Table 1: Phase transition temperatures and latent heats for compounds **1**-n and **2**-n.

Compounds	Phase transition temperatures (ºC)							Latent heats (kJ mol^{-1})		
	C		SmC		SmA		I	mp	SmC–SmA	SmA–I
1-4	•	69	–		–		•	62.6		
1-6	•	77	–		•	91	•	37.0		6.5
2-4	•	90	•	118	•	216	•	16.8	2.6	8.7
2-6	•	>250	–		–		•	decomp.		

C, SmC, SmA and I indicate crystal, smectic C, smectic A and isotropic liquid phases, respectively.

Acknowledgements: This work financially supported by JSPS KAKENHI [22H03781], JST SPRING [JPMJSP2111], and Paloma environmental technology development foundation.

References:
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Synthesis of Photoactive Dimers with 1,3,4-Thiadiazole Cor Unit

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Keywords: 1,3,4-Thiadiazole, Photoisomerization, Heterocycle Liquid Crystal, Fluorescence.

Currently, there is a constant search for new materials, and molecular materials have been the focus of research for years. Of interest are photoactive materials, which include groups such as cyanobiphenyl and azobenzene; and liquid crystals, which present an intermediate state between solid and liquid, and are favored by the incorporation of heterocycles such as 1,3,4-thiadiazole to the molecules[1-3].

In this work, four new final compounds derived from 1,3,4-thiadiazole were synthesized and organized in two series incorporating cyanobiphenyl and azobenzene photoactive units, with series **D1** having as connection to the rigid center an ester group and series **D2** an ether group. These compounds were characterized by infrared spectroscopy and NMR ^{1}H and ^{13}C, and their thermal and mesomorphic properties were determined by polarized light optical microscopy and thermogravimetric analysis. Finally, their optoelectronic properties were studied by photoisomerization study for azo groups and fluorescence for cyanobiphenyl groups.

The compounds of both series exhibited enantiotropic thermotropic-type liquid crystal properties with wide mesomorphic ranges and the characteristic photoactivity of each group.

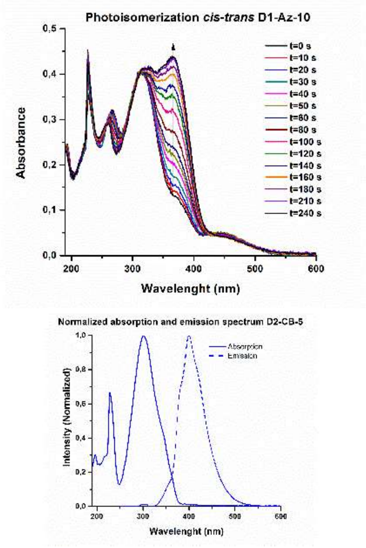

Figure 1: Compound synthesized and photophysical study.

Acknowledgements: FONDECYT 1231767

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Thiadiazole derivatives polycatenar systems: synthesis, characterization and functional properties evaluation

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Keywords: columnar, thiadiazole, oragnogelator

Polycatenar liquid crystals are unique due to their distinctive polybranched structure which allows generating an array of liquid crystalline phases, providing a significant level of adaptability. [1] These polycatenar liquid crystals can be tailored to respond to different stimuli such as light, temperature, and electric or magnetic fields. This characteristic makes them appealing for incorporation into smart materials and devices.[2] In this work, polycatenar mesogens containing 1,3,4-thiadiazole heterocyclic units were synthesized and characterized. The compounds shown photoluminescent, organogelator π, and columnar liquid crystal properties. The characterization of the precursors and final compounds was carried out using FT-IR, ^{1}H and ^{13}C NMR. The mesomorphic and thermal properties were studied by Polarized Light Optical Microscopy (POM), Differential Scanning Calorimetry (DSC) and Thermogravimetric Analysis (TGA). The photoluminescent properties were studied by UV/Vis and fluorescence spectroscopy. Organogelators properties were examined in different solvents, exhibiting notable solvatophotochromism that has potential use as a sensor.

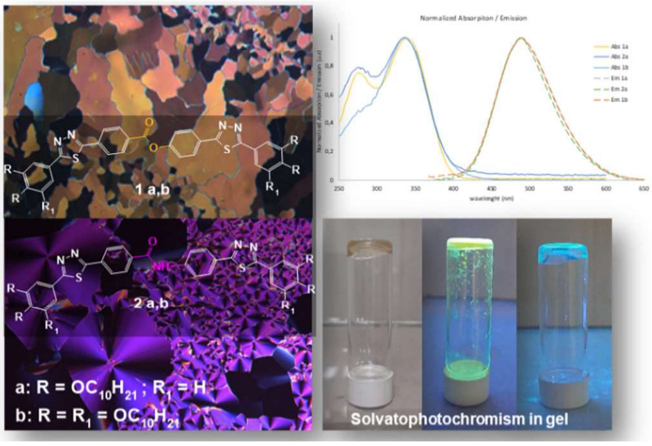

Figure 1: Molecular structure, textures, absorption and emission and organogelator behavior in different solvents

Acknowledgements: The authors thank to FONDECYT 1221631 and 1231767 project for the funding provided to carry out this research.

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To Fluorinate or not to Fluorinate ? – Strategies Towards Luminescent Merocyanine Liquid Crystals

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Keywords: merocyanines, liquid crystals, luminescence, fluorophobic effect

Merocyanines are an important class of donor-acceptor dyes, which are used for chemosensors, biomolecule targeting, photovoltaics, photoswitches and many other applications [1]. Although several liquid crystalline (LC) merocyanines are known, it remains a challenge to combine good absorption and emission properties with the formation of stable mesophases. In order to tackle this challenge, we combined molecular features of merocyanines with good dye, but poor LC properties [2] with merocyanines showing poor dye, but good LC self-assembly [3]. The role of side chain fluorination in order to obtain merocyanines with the desired properties will be discussed [4].

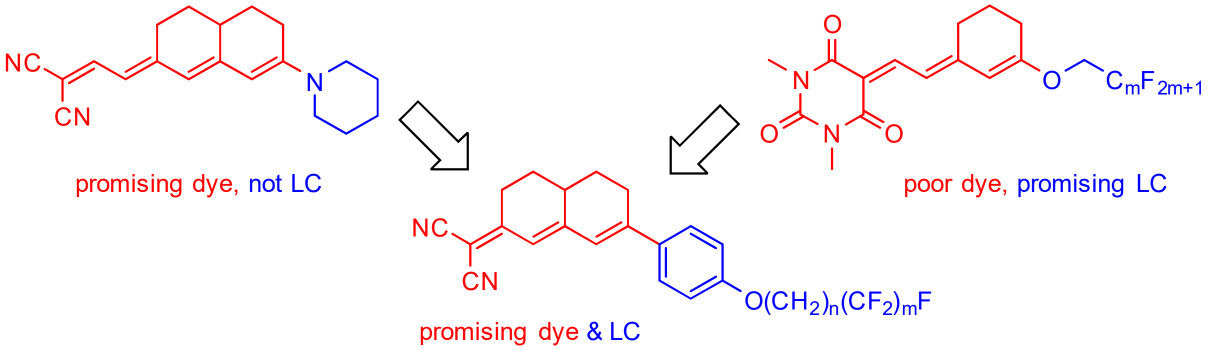

Figure 1: Design of merocyanines, which combine good dye characteristics with stable LC mesophases

Acknowledgements: This work was funded by DFG (LA907/20-1, SNAPSTER) and DAAD -Procope (PLISE).

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Treasure Trove Soft Materials Derived from Cholesterol

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Keywords: Sterol, chirality, frustrated phases, technically significant phases, unprecedented sequences, reentrant phenomenon, incommensurate structures, and glassy/frozen state

An account of the historical aspects and the state-of-the-art of chiral liquid crystal (LC) dimers derived from naturally occurring, pro-mesogenic cholesterol (cholest-5-en-3β-ol) will be presented. We will discuss the influence of cholesterol on the thermotropic LC behavior of nonsymmetric dimers where it is covalently tethered to the different conventional calamitic cores through the flexible spacer of varying length and parity. Apart from imparting the chirality, it facilitates such dimers to not only exhibit rich mesomorphism, unusual sequences, fluid incommensurate structures, highly frustrated phases, reentrant phenomenon, and technically significant mesophases but also it helps in widening the thermal width of mesophases. Besides, it typically freezes the mesophase into a glassy state. The unprecedented platform cholesterol provides in realizing such exceptional phase transitional characteristics stems from its unique steroid skeleton, rigidity, bulkiness, and conformation/length of the terminal hydrocarbon tail attached. The talk also covers a perspective on the future scope, opportunities, and challenges in these truly advanced functional soft materials.

Tris(*N*-phenyltriazole) and 1,3,4-oxadiazole – a promising combination for star-shaped luminescent Discotic Liquid Crystals

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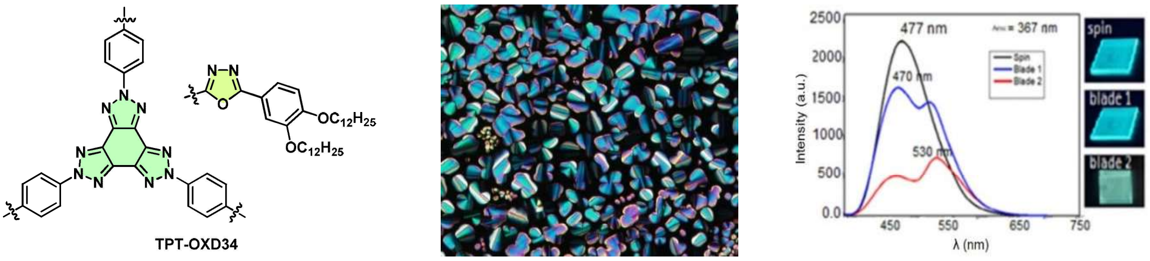
Keywords: Tris(*N*-phenyltriazole), 1,3,4-oxadiazole, Discotic Liquid Crystal, Luminescence

Discotic Liquid Crystals (DLCs) remain a focal point of interest owing to their notable self-organization capabilities, versatile applicability, and well-established one-dimensional conduction. However, there is still a significant unexplored territory. In our pursuit of novel cores for this material class, our group successfully synthesized the first DLC derived from the Tris(N-phenyltriazole) core (TPT), which only presented an unstable monotropic $\mathrm{Col_h}$ phase [1], but was later stabilized through structural changes carried out by Dhingra et al [2]. To further assess the efficacy of this core, we investigated its synergistic combination with the 1,3,4-oxadiazole heterocycle—an extensively used heterocycle in the development of liquid crystals and luminescent materials (Fig. 1a). The material displayed impressive $\mathrm{Col_h}$ mesomorphism extending from room temperature to 339 °C, as confirmed by POM (Fig 1b), DSC and XRD. In solution, it presented fluorescence quantum yields close to 100%, which dropped to values between 43 and 38% when in the form of thin films, depending on the deposition technique used (Fig 1c). Although the films deposited by spin-coating and blade-coating showed different morphologies by AFM, in the diode-type devices the electrical responses were similar, presenting three conduction regimes, ohmic, SCLC-trap limited and the trap-filling regime. In a simple OLED structure, the spin-coated film of the LC exhibited electroluminescence with an emission maximum at 500 nm. The results show that the combination between TPT and oxadiazole is very promising, both from a mesomorphic point of view, as well as from a photophysical and application point of view.



(a) (b) (c)

Figure 1: (a) Structure of the compound investigated in this study; (b) Representative texture of the $\mathrm{Col_h}$ phase; (c) Thin films emission spectra and picture.

Acknowledgements: CNPq, CAPES, INCT-INEO, INCT-Catálise and UFSC.

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A2

Ionic liquid crystals

How do ionic superdiscs self-assemble in nanopores?

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Keywords: Confinement, Discotic ionic liquid Crystals, Alignment

Discotic Ionic Liquid crystals (DILCs) are known for their high conductive properties along the columnar axis[1]. However, unlike non-ionic DLCs electric-field-induced orientation of the columns of DILCs, necessary for application in e.g. photonic devices, is not possible[2]. An alternative pathway to achieve highly ordered columnar mesophases for DILCs is confinement in a rigid scaffold, which provides structure. In a previous study we observed the alignment of non-ionic DLCs upon confinement in the pores of membranes[3]. Therefore, in this project we investigated the influence of cylindrical confinement for DILCs. For this purpose, DOPA-based Ionic Liquid Crystals were prepared: Three alkyl groups of varying length were attached to the aromatic core motif, which was functionalized with a cationic cyclic or acyclic guanidinium headgroup. These ILCs were imbibed into the cylindrical pores (ø = 180 nm) of anodic aluminum oxide membranes. The resulting metamaterial showed a rich phase behavior, which deviates from the bulk mesomorphic properties of the liquid crystalline component, including transitions between axial and radial alignment depending on the hydrophobicity of both the membrane and the ILC.

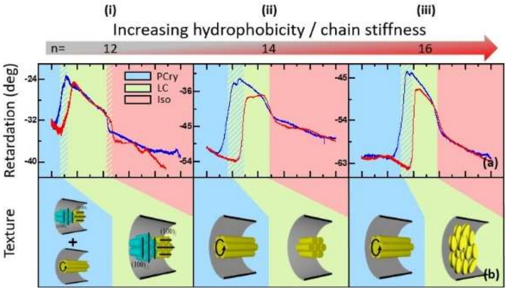

Figure 1: Texture formation of DOPA-ILCs within the pores

Acknowledgements: We acknowledge funding by the Deutsche Forschungsgemeinschaft (DFG). We thank the Deutsche Elektronen-Synchrotron DESY and the European Synchrotron Research Facility ESRF for beamtime.

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Imidazolium based benzoate carboxylates

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Keywords: ionic liquids, liquid crystals, mesophase, mesogene

Ionic liquids (Ils) and ionic liquid crystals (ILCs) are promising compounds in the field of material science. Due to their tailor-made properties they can be used as solvents[1-3], catalysts[4] as well as for electrochemical conductivity[5]. Our work deals with imidazolium based benzoate carboxylates as potential ionic liquid crystals. The liquid crystalline behavior of the respective target molecules was investigated using polarized optical microscopy (POM), differential scanning calorimetry (DSC) and X-ray diffraction (XRD). Our main question focuses on the dependence of the liquid crystalline properties on the chain length and the occurrence of an odd-even effect.

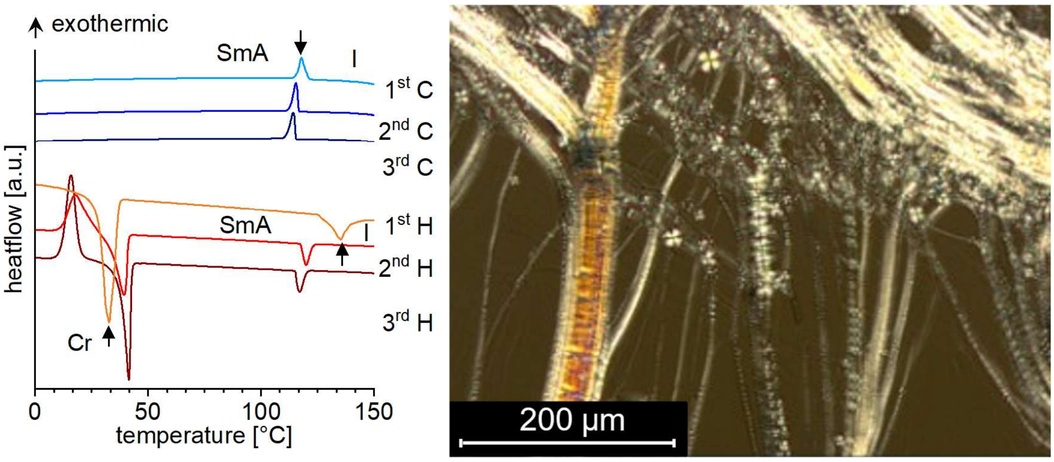

Figure 1: On the left the a DSC thermogramm; on the right maltese crosses are shown.

Acknowledgements: We acknowledge the Carl Zeiss Stiftung, the Ministerium für Wissenschaft Forschung und Kunst des Landes Baden-Württemberg, the Carl-Schneider-Stiftung Aalen and the Deutsche Forschungsgemeinschaft for their financial support.

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Mesophase stabilization in ionic liquid crystals: new insights from solid-state NMR

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Keywords: ionic liquid crystals, hydrogen bonding, diffusion, nuclear magnetic resonance.

The mesophasic behavior in ionic liquid crystals (ILCs) is governed by a delicate balance between hydrogen bonding, electrostatic interactions, and dispersion forces. We apply solid-state and diffusion NMR techniques [1] combined with DFT computational analysis to understand the roles and relative contributions of these interactions in ionic mesophase stabilization.

Our experimental data in different classes of ILCs revealed the trends in the orientational order and phase stability in ionic liquid crystals depending on cation structure and anion properties and shed light on the mechanism of layered structure stabilization from the perspective of molecular-level dynamics [2-7]. In single-chain monocationic ILCs, the order parameter *S* has been found to correlate with physicochemical properties of anions and increase with a mesophase stability range [2]. On the other hand, an expanded hydrogen bonding network in hydrated ILCs results in higher phase stability with an accompanying decrease in the orientational order [3]. Thus the role of anisotropic alignment of cations and the contribution of dispersion forces in the mesophase stability decreased upon hydration. Anisotropy of translational diffusion increased in the hydrated samples, supporting the layer-stabilizing effect of hydration [4]. In double-chain ILCs, the enhanced contribution of van der Waals interactions led to a greatly increased order parameter [5]. On the other hand in dicationic ILCs, we found that the side-chain ordering and the alignment of imidazolium rings are similar to those in analogous single-chain monocationic analogues [6]. To explain this finding, we hypothesized that the presence of a dynamic spacer effectively “decouples” the motion of two imidazolium moieties. NMR data obtained in bulk ILCs in isotropic, liquid-crystalline, and solid states has shown that the dynamic state of ions ranging from high reorientational and translational freedom to partial orientation and positional order to full immobilization, respectively, has no dramatic effect on cation–anion hydrogen bond strength [7]. On the other hand, nanoconfinement of ILCs led to local disruption of hydrogen bonding due to competing interactions of anions with solid interfaces.

Acknowledgements: This work was supported by the Swedish Research Council VR.

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New ionic mesogens based on a cyanoborate building block and lipophilic or hydrophilic counter ions

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Keywords: Non nucleophilic borate mesogens, Ionic liquid crystals, Ion conduction, Electron density reconstruction, Solid-state NMR

Ionic liquid crystals (ILCs) are intensely investigated as future electrolytes,[1] which can be subsequently immobilised by polymerisation.[2] However, conductivities which are interesting for applications > 10^{-3} Scm^{-1} are rarely achieved. This prompted us to test robust, non-nucleophilic cyanoborates immobilised on an mesogenic residue as anionic part of the ILC, combined with either lipophilic sodium or potassium crown ether cation complexes or the lipophilic tetrabutylammonium ion (Figure).[3] The structure of the bilayer SmA phases are uncovered in detail by X-ray scattering and solid-state NMR techniques. This study shows the rather low density in the ionic subphase of the layered LC promoting the rather high conductivity values found by electrical impedance studies of this single-ion conductor. Values of the correctly aligned phases approach 10^{-4} Scm^{-1} in the SmA phase at 85 °C and 10^{-5} Scm^{-1} at 40 °C, which are among the highest found for crown ether materials. These findings are attributed to the low densities of the ionic nanophases and the low nucleophilicity of the borate anions.

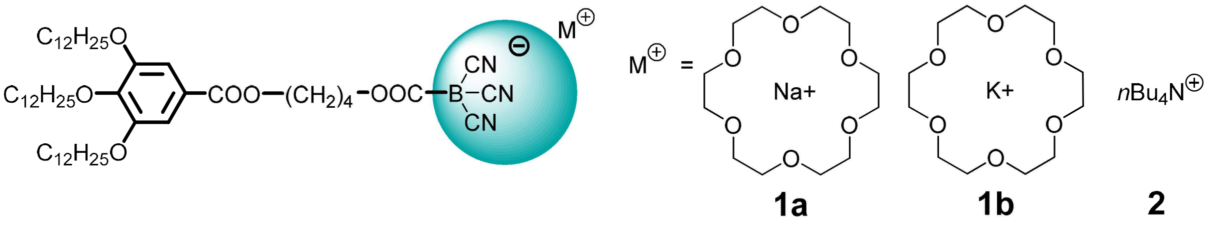

Figure. Structure of the new cyanoborate ILCs **1** and **2**.

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Non-symmetric dimeric luminescent ionic liquid crystals with FRET phenomenon

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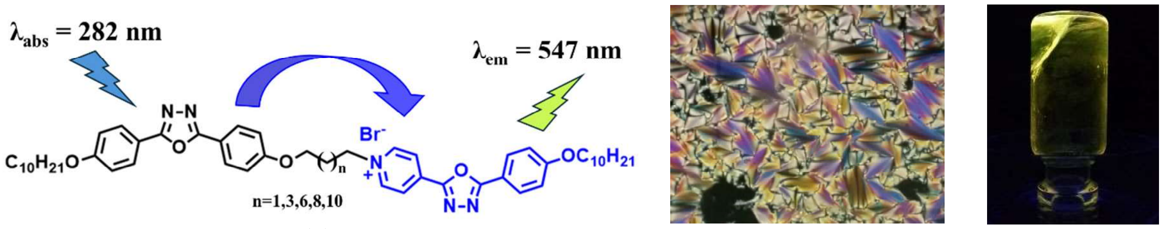
Keywords: Ionic Liquid Crystals, non-symmetry, dimers, FRET, 1,3,4-oxadiazole

Ionic Liquid Crystals (ILCs) can be considered materials that combine the properties of liquid crystals and ionic liquids, where the explicit charges favour changes in the self-assembly capacity and type of molecular organization of the material due to nanosegregation through strong coulombic interactions.[1,2] Considering the importance of this class of materials and its vast and differentiated applications possibilities, five new non-symmetric ionic dimeric Liquid Crystals with different alkyl spacer were synthesized and investigated (Fig. 1a). The non-symmetric structure was planned also intending to investigate how the material prefers to self-organize when there is competition in the interaction between the different parts of the non-symmetric molecule (ionic and non-ionic), increasing understanding of this class of materials. All five molecules presented liquid crystalline behaviour with enantiotropic SmA (Fig. 1b) phase at temperatures above 100 °C and normally showing a large range of mesomorphism. Preliminary XRD data indicates that, for these materials, the molecular organization in the SmA phase leans towards a randomized distribution of the aromatic and ionic cores, contrary to the expected prevalence of coulombic interactions. Due to the presence of the 1,3,4-oxadiazole heterocycle, the materials showed luminescence, with a difference in behaviour between the ionic and non-ionic arms,[1] favouring Förster's Resonant Energy Transfer (FRET) phenomenon between the non-ionic (donor) and the ionic one (acceptor) (Fig. 1a). The materials also presented the formation of luminescent gels (Fig. 1c), which further expand its relevance and applicability, being able to form conductive gels and fibers, resulting in application in LECs (light-emitting electrochemical cell), for example.



(a) (b) (c)

Figure 1: (a) Structure of the non-symmetric ionic dimmers synthesized, with the representation of the FRET process; (b) Typical SmA texture observed for all compounds; (c) Gelation process observed for some compounds.

Acknowledgements: CNPq, CAPES, INCT-INEO, UTFPR, UFSC.

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Potential Utility of Zwitterionic Liquid Crystals for the Design of Functional Bicontinuous Cubic Liquid Crystals

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Keywords: Bicontinuous Cubic Phase, Gyroid, Zwitterion, Proton Conduction, Ionic Liquid

Bicontinuous cubic ($\mathrm{Cub_{bi}}$) phase is a kind of nano-segregated liquid-crystalline (LC) phases in which both of two incompatible molecular parts form 3D continuous domains.[1] It has been found that $\mathrm{Cub_{bi}}$ phases appear between lamellar and columnar phases both in the case of lyotropic liquid crystals and thermotropic ones. The volume balance between the two incompatible parts is one of the critical parameters for designing liquid crystals forming $\mathrm{Cub_{bi}}$ LC assemblies. To date, we have focused on ionic liquid crystals having zwitterionic headgroups.[2,3] For example, we designed and synthesized pyridinium-based amphiphiles having zwitterionic headgroups. Although it forms only layered smectic phases in the pristine states, it co-organized into $\mathrm{Cub_{bi}}$ LC phases in the presence of bis(trifluoromethane)sulfonimide ($\mathrm{HTf_2N}$) [3] It can be explained by the formation of ion pairs between the pyridinium zwitterion part and $\mathrm{HTf_2N}$ through an ion exchange and the increase of the volume of the ionic parts. The obtained LC material shows high ionic conductivity. Based on the molecular design of the amphiphilic zwitterions, we have recently succeeded in the development of a gemini-type amphiphilic zwitterion monomer forming $\mathrm{Cub_{bi}}$ phases.[4] UV irradiation for the monomer in $\mathrm{Cub_{bi}}$ phases leads to the formation of self-standing and insoluble polymer films with preserving the gyroid nanostructures. The polymer film shows quite high ionic conductivity in the order of 10^{-2} S $\mathrm{cm^{-1}}$ in the H_2O-absorbed condition.

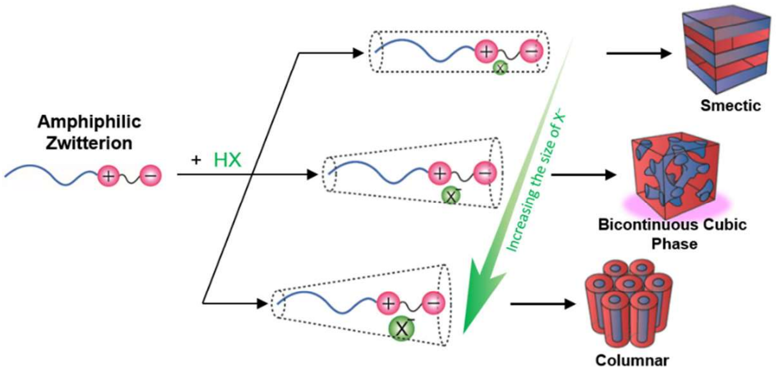

Figure 1: Our design strategy for functional bicontinuous cubic liquid crystals.

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A3

Nanostructured systems

Differential Dynamic Microscopy to Characterise Viscoelastic Ratios of Lyotropics

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Keywords: Lyotropic, chromonic, nematic, elastic constant

Characterising the elastic constants of lyotropic liquid crystals is notoriously difficult due to the impracticality of applying electric fields, causing movement of charged entities in the solvent. During this project, we set out to determine the range of viscoelastic ratios (K/η) using Differential Dynamic Microscopy (DDM) [1] for lyotropic nematic liquid crystals, for the first time. Thus, we demonstrate that a standard microscope can be used to measure the viscoelastic properties of lyotropic liquid crystals. This approach is an effective alternative to light scattering and avoids any requirement to apply an electric field. DDM allows for the extraction of scattering information directly from high-speed microscope images. Dynamic analysis of images from different polariser geometries is performed, providing the splay, twist and bend viscoelastic ratios. This method offers a practical solution using a standard microscope with polariser and analyser sets. We demonstrate results with the lyotropic chromic liquid crystal, sunset yellow (SSY), and a standard reference 5CB.

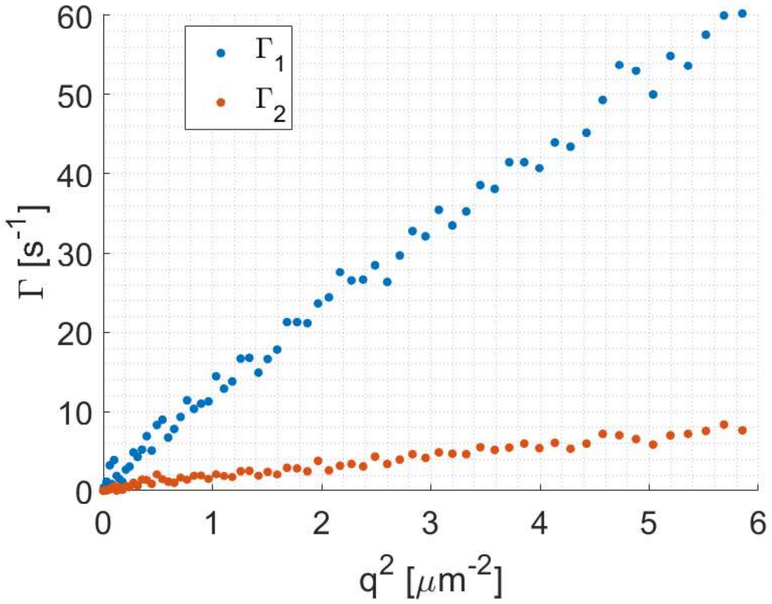

Figure 1: Relaxation rates, Γ_1 and Γ_2, for 28wt% SSY in water, with the gradient of each slope giving the splay and twist viscoelastic ratios respectfully.

Acknowledgements: This work was funded by BBSRC in collaboration with IBioIC and Marine Biopolymers Ltd.

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Flow-induced Assembly of Graphene and Graphene Oxide Liquid Crystals

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Keywords: Graphene, Liquid Crystals, Shear Stress, 2D Materials, Ordering

Graphene and graphene oxide (GO) are two-dimensional materials with metallic and semiconducting properties, respectively. Graphene is a one-atom-thick layer of graphite, and its flakes have extremely large aspect ratios. Water-dispersible GO has still very large aspect ratio flakes, and its dispersions can form a nematic liquid crystal at relatively low concentrations. The size distribution, shape and chemical composition of GO flakes vary depending on the preparation conditions, such as the nature of the precursors and the chemical reactions during the synthesis. Colloidal dispersions of graphene can be obtained by chemical reduction of GO dispersions, but the reduced-graphene oxide flakes often have many defects that influence the mechanical and conductive properties of the flakes. An alternative route is the mechanical exfoliation of graphite and, as for GO, the colloidal dispersion properties depend on the specificities of the preparation method. The liquid crystal phase formation is affected by various factors such as concentration, shape, functional groups, and aspect ratio. The lateral size of the GO flakes affects also macroscopic optical properties [1]. In addition to the phase formation and related birefringence, affected by the aspect ratio, and chemical composition of GO flakes, the macroscopic optical properties are determined by the macroscopic alignment, obtained by e. g. shearing. Interestingly, optical features at bulk scale were reported to be originated by positional order [2, 3], thus the macroscopic ordering is relevant for the study of different types of graphene liquid crystals. We have realized dispersions of single/ multi-layers graphene in solvents, and we will report the behaviour under shear stress conditions, comparing with various GO liquid crystals. The flow-induced organization will be presented correlating it to the lateral dimension and aspect ratio of the flakes. The characterization of the graphene liquid crystals is carried out with various optical methods and the aspect ratio and shape determination is achieved by scanning and atomic force microscopy. Ability to tune the macroscopic optical properties by applying a shear stress opens a path to the development of feasible, energy efficient applications of graphene liquid crystals with highly sensitive response to external stimulation in areas such as advanced electronics, chemical, bio, and physical sensing.

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Liquid Crystallinity and Optical Properties of Colloidal Nanohybrids

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Keywords: Colloidal liquid crystals, Inorganic/organic hybrids, Structural colors

Structural colors have attracted attention for sustainable optical materials. These colors are originated from selective light reflection and diffraction of periodic several hundred nm structures. Self-assembly of liquid crystals to form periodic structures is effective process for developing structural color materials[1]. Molecular-based cholesteric liquid crystals with helical pitch are typical examples of structural materials. Some liquid-crystalline colloidal nanoparticles dispersed in solvents also exhibit structural colors such as cellulose nanocrystals[2], inorganic nanorods[3] and inorganic nanosheets[4]. We have synthesized various inorganic/polymer hybrid colloidal liquid crystals as functional materials[5-9]. Here, we report new photonic colloidal liquid crystals composed of mineral/polymer hybrid rods and water. The colloidal liquid crystals exhibited high reflectance and strong angular dependency. The coloration was tuned by control of particle concentration and particle size. In addition, the colloidal liquid crystals were immobilized in organic polymer network, which exhibited mechanochromic properties with angular dependency.

Acknowledgements: This work was supported by JSPS KAKENHI Grant Numbers JP19H05714, JP19H05715 and JP22K14562.

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Novel Organic-Inorganic Hybrid UV Photodetectors Based on Zinc Oxide Nanorods and Polymer-Dispersed Cholesteric Liquid Crystals

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Abstract

A high-performance ultraviolet (UV) photodetector was successfully fabricated by employing polymer-dispersed cholesteric liquid crystal (PDCLC) as a sensitization agent on a zinc oxide nanorod (ZNR) heterostructure. The ZNR film was synthesized via hydrothermal technique and subsequently coated with PDCLC. The incorporation of PDCLC significantly enhanced both the electrical and optical performance of the heterojunction UV photodetector. Compared to devices based solely on ZNR film or zinc oxide seed layer, the PDCLC-decorated ZNR film-based UV photodetector exhibited a superior photocurrent density of 171 $\mu A/cm^2$ at 10 V under 5 mW/cm^2 of UV light (365 nm). The sensitization by PDCLC facilitates the activation of charge carriers in zinc oxide, promoting the alignment of energy bands through a spontaneous and time-correlated transient response. The device demonstrated an outstanding responsivity of 170.51 mA/W at 10 V, along with a remarkably high external quantum efficiency of 57.44% at the same voltage. In contrast, devices based on ZNR film or zinc oxide seed layer exhibited significantly lower responsivity (72.07 mA/W and 7.26 mA/W, respectively) and external quantum efficiency (23.09% and 2.4%, respectively). These results underscore the potential of PDCLC/ZNR heterostructures in the development of efficient UV photodetectors.

Key words: UV Photodetector, ZnO NRs, Polymer dispersed Cholesteric liquid crystal, Photocurrent

Acknowledgements: The authors thank the Central Research Instrumentation Facility (CRIF) and the Department of Physics at NIT Warangal for providing support in furnishing the necessary research facilities. S.P. Ramadevi, the author, was granted financial support by the CSIR (Government of India) in the form of a senior research fellowship (09/0922(0012)/2019-EMR-1).

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2. Energy saving, transparency changing thermochromism in dye-doped cholesteric liquid crystals for smart windows. **Ramadevi Suguru Pathinti,** Buchaiah Gollapelli, Saumya Ranjan Pradhan, Jayalakshmi Vallamkondu. Journal of Photochemistry & Photobiology, A: Chemistry 444 (2023) 114981.
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Perfect restacking of 2D-materials from their liquid-crystalline nanosheets suspensions

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Keywords: lamellar phase, colloids, nanosheets, cation exchange, first-order phase transition

Aqueous suspensions of $H_3Sb_3P_2O_{14}$ mineral nanosheets are one of the rare examples of colloids based on 2D materials exhibiting a lamellar liquid crystalline (LC) phase [1,2]. Because the lamellar period can reach several hundred nanometers, the suspensions show vivid structural colors and because these colors are sensitive to various chemicals, the suspensions can be used as sensors [3]. Such applications require the well-ordered deposition of the nanosheets from suspension to prepare solid-state devices. We report here the crystalline restacking of the layered $H_{3(1-x)}M_{3x}Sb_3P_2O_{14}$, (where M = Li, Na, K, Rb, Cs and $0 \leq x \leq 1$) dielectric materials from their nanosheets dispersed in colloidal LC suspension, induced by a simple pH change using alkaline (MOH) bases [4]. Using polarized-light microscopy and X-ray scattering, we show that thanks to the lamellar LC order of the colloidal suspension, the restacking is highly accurate and avoids the turbostratic disorder of the nanosheets classically observed with other 2D materials. Strikingly, the restacking process exhibits features highly reminiscent of a first-order phase transition, with a phase coexistence region where both ~ 1 nm and ~ 120 nm lamellar periods are observed simultaneously, which we have described theoretically. This crystalline restacking of nanosheets from their lamellar LC suspensions opens the way to the production of complex integrated electronic, spintronic or photonic structures.

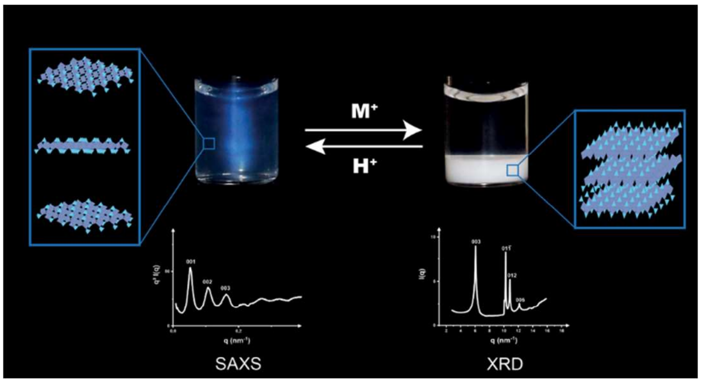

Figure 1: Crystalline restacking (right) of the 2D phosphatoantimonic $H_{3(1-x)}M_{3x}Sb_3P_2O_{14}$ materials from their nanosheets dispersed as a colloidal lamellar LC suspension (left), induced by a simple pH change using alkaline bases.

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Two-dimensional vermiculite liquid crystalline dispersion: Giant electro-optical Kerr effect and magneto-optical Cotton-Mouton effect

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Keywords: 2D materials, clay minerals, vermiculite, lyotropic liquid crystalline dispersion, electro-optical Kerr effect, magneto-optical Cotton-Mouton effect

Lyotropic liquid crystalline dispersion based on exfoliated layered clay minerals has been discovered for a century, while the research is hindered by its insensitive field-induced alignment and resultant poor optical response. Here, we report a two-dimensional vermiculite liquid crystalline dispersion (2D VMT LC for short). 2D VMT LC shows both a giant electro-optical Kerr effect and magneto-optical Cotton-Mouton effect, where the Kerr coefficient and Cotton-Mouton coefficient, i.e., the sensitivity descriptors, respectively reaches 10^{-4} m V^{-2} and 10^3 m^{-1} T^{-2}, achieving the record-high level in all the Kerr and Cotton-Mouton media. These giant effects are ascribed to the extremely large geometrical anisotropy of 2D VMT with an aspect ratio of $>10^3$ and the inherent electric dipole and magnetic susceptibility anisotropy. Notably, the inherent electric dipole is reported for the first time and leads to the discovery of 2D ferroelectricity in VMT. These finding inspires the research on developing new LC materials and studying their electro-optical and magneto-optical properties.

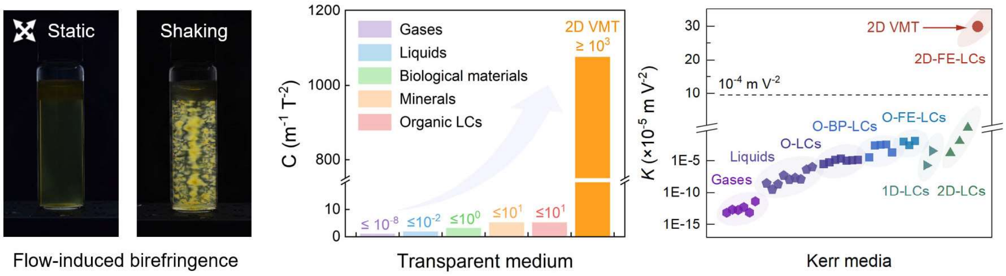

Figure 1: 2D VMT LC and its giant field-induced response.

Acknowledgements: This work is supported by the National Natural Science Foundation of China (Nos. 51920105002, 52125309, 52273311, 51991343, 51991340, and 52188101), Guangdong Innovative and Entrepreneurial Research Team Program (No. 2017ZT07C341), Shenzhen Science and Technology Program (Nos. WDZC20200819095319002, JCYJ20190809180605522, JCYJ20220818100806014, WDZC20231128154552002), and Shenzhen Pengrui Young Faculty Program (No. SZPR2023002).

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Variable-dimensional reactor (VDR) for morphology control of multiple nanomaterials and their applications

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Keywords: Hyperswollen lamellar phase, dimensionality, nanomaterials, reactor

Nanomaterials have many unique improved properties: surface area (S_{ext}), catalytic performance and electrical conductivity (σ). By using soft template approaches we can synthesize a wide range of nanomaterials with different morphologies in mild conditions.

We first established the synthetic capabilities of hyperswollen lamellar phases as soft templates [1]. This allows us to develop the two-dimensional reactor in amphiphilic phases (TRAP) method, with a low-cost surfactant and scalable potential [2, 3]. The specific mixtures of these amphiphilic molecules and solvents form soft sheet-like templates (lyotropic liquid crystals), in which we were able to synthesize nanosheets of various materials [4-6].

In some specific ternary mixtures, surfactants can be dispersed into a specific orientation, creating variable-dimensional reactor (VDR) in-between the different ordering limits of liquid crystals and isotropic liquids. In addition, we can choose whether the solvent inside and outside the surfactant templates will be water or an organic solvent. Hence the VDR can be hydrophilic or hydrophobic, respectively.

This characteristic polymorphism allowed us to establish a multi-dimensional synthetic process to tune different parameters such as hydrophilicity, mixture concentration [7] and synthesis conditions that allow us to obtain a wide range of nanomaterials with different morphologies. Up to date we have been able to synthesize a wide range of aluminosilicates compounds, metal oxides and polymers, which can also be further utilized as supports or precursors for new materials.

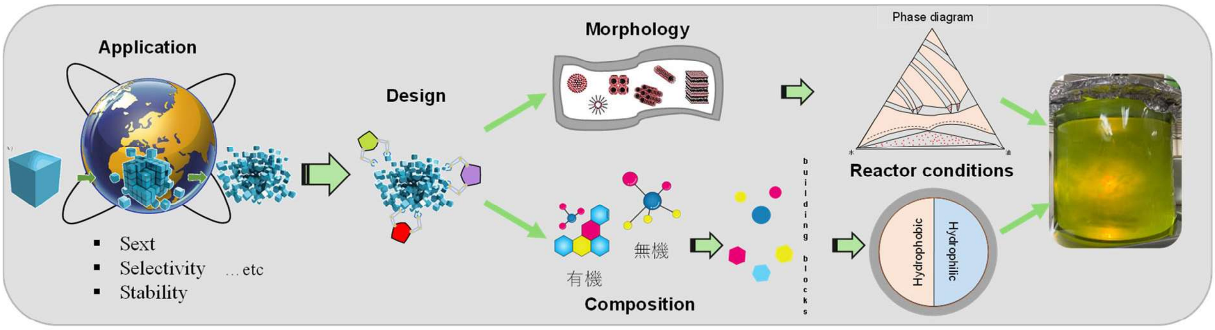

Figure 1: Schematic illustration of VDR method.

Acknowledgements: JSPS KAKENHI (JP22H04477, JP22H02158)

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Electronic molecular materials

Optical and Electronic Properties of Discotic Liquid Crystalline Metalloporphyrins

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Keywords: Porphyrin, Metallopophyrin, Organic Semiconductor, OTFT

Organic semiconductor and OTFT based sensor is a flexible and sensitive sensors applicable for glucose, VOCs, gas, and bio/medical detection. The OTFT sensor does have the down side that its function gradually declines when exposed to the atmosphere, water, or chemical components, but a chemical sensor can be created using these characteristics. The porphyrin molecules have stable structure regarding light, acids, base, and electrical condition, and complex formation with various metal ions are possible as an organic semiconductor material with 18 π conjugated electrons. The synthesis was conducted such as these, alkyl chain was used to give liquid crystallinity to the sides, π electron expanders were placed for the characteristics of high mobility at the middle. In this work, we report to research of the metalloporphyrin regarding each liquid crystallinity behavior, optical and electrical properties in accordance with the various changes to the central metals.

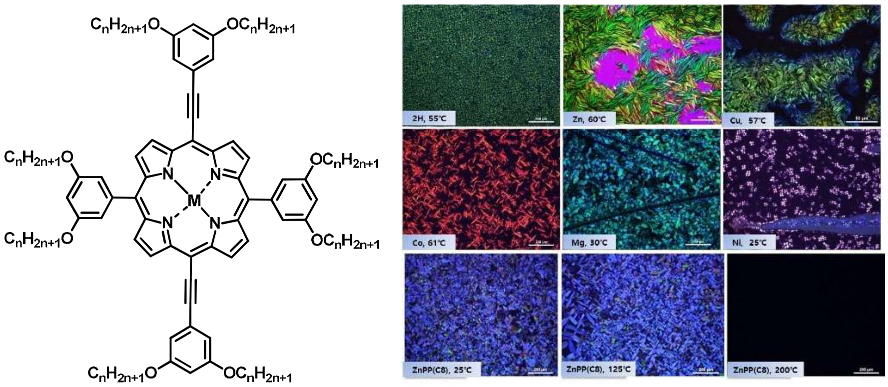

Figure. Metalloporphyrin structure and their POM images

Acknowledgements: This work was supported by the Technology Innovation Industrial Program funded by the Ministry of Trade, Industry & Energy (10052667, Korea).

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Perylene diimide columnar liquid crystal with spin-coated and blade-coated thin films from toluene solvent

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Keywords: Organic semiconductors, columnar liquid crystals, blade coating, spin coating

Liquid crystals (LC) are materials which present intermediate phases between the crystalline solid and the isotropic liquid and are promising organic semiconductors for presenting self-organization and the possibility of molecular alignment on electrodes, providing greater mobility of charge carriers[1,2] and the self-healing of structural defects in the mesophase reduces the charge-traps. In this work, we present the characterization of a thermotropic discotic LC (designated BPD-11) derived from benzoperylene diimide with a hexagonal columnar mesophase at room temperature and investigate its properties in thin films produced by spin coating and blade coating techniques using toluene as solvent. The mesomorphic characterization of the material was performed by polarizing optical microscopy (POM), differential scanning calorimetry (DSC), thermal gravimetric analysis (TGA) and x-ray diffraction (XRD). The morphological, optical, and electrical properties of the films were performed and compared for both film deposition techniques. The results indicated that these films are very attractive for optoelectronic devices applications such as in OLEDs and solar cells.

Acknowledgements: CNPq, CAPES-COFECUB, INCT/INEO, FAPESC, OCTA and UFSC.

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Pseudo-Dielectric Relaxation in NOA65 Incorporated with an Azobenzene Dye

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Keywords: NOA65, Azo dye, *Trans*–*cis* isomerization, Pseudo-dielectric relaxation.

The booming LC research and development highlights the importance of materials like polymer and dyes for enhancing LC characteristics. Önsal *et al*. conducted an in-depth study on the effects of incorporating different dye concentrations into polymer-dispersed LC [1]. While existing literature predominantly focuses on the interactive effects among polymer, dyes, and LCs, this study specifically explores the dielectric behavior of dye-doped polymer in a capacitor cell [2], utilizing an empirical modification of the Debye relaxation. The slow *cis*–*trans* isomerization process of the dye is observed at low frequencies. The results at a fixed frequency of 20 Hz reveal minimal permittivity variation of the photopolymerized NOA65 doped with 2.0-wt.% a bis-azobenzene dye (ChAD-3C) as shown in Fig. 1(a). Complex dielectric spectra of the doped polymer are analyzed using a two-relaxation Havriliak–Negami model, accounting for the asymmetry and broadness of the dielectric dispersion curve (Figs. 1(b) and (c)). Preliminary findings suggest that the composite's dielectric relaxation undergoes a blueshift as temperature T rises, causing overlap with the pesudo-dielectric signal. Figure 1(c) shows the observed pseudo-dielectric relaxation at ~200 kHz is a result of the superposition of two signals.

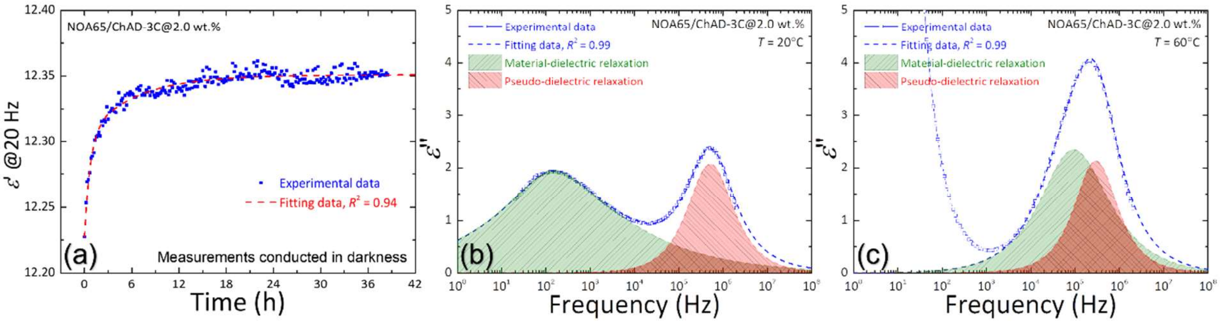

Figure 1: (a) Time-evolved minute ε' variation at 40 °C and (b) f-dependent ε'' function and the fitting curves using the two-relaxation H–N model at T = 20 °C and (c) T = 60 °C. The ChAD-3C-doped NOA65 prepolymer was exposed to 13.4-mW·cm^{-2} ultraviolet light (at 365 nm) for 3 min to form polymer.

Acknowledgement: National Science and Technology Council, Taiwan.

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The development of π-conjugated compounds exhibiting polar smectic phases for improving the characteristics of bulk photovoltaic effect

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Keywords: π-Conjugated liquid crystals, Ferroelectric liquid crystals, Ferroelectric bulk photovoltaic effect.

Polar molecular assemblies of chiral π-conjugated liquid crystals are essential for functional expression of a bulk photovoltaic effect (BPVE).[1] The BPVE is a characteristic phenomenon which is different from conventional photovoltaic effect based on the p-n heterojunctions because the output voltage is independent from the bandgaps of semiconductors and the work functions of electrode materials. However, the output characteristics of BPVE in the polar liquid crystalline materials achieved thus far have been unsatisfactory. Therefore, we are currently addressing the improvement of the open-circuit voltage, short-circuit current and energy conversion efficiencies of the BPVE. In this study, we synthesized several chiral π-conjugated compounds (Figure 1).[2] Their liquid crystallinity was evaluated by polarizing optical microscopy, differential scanning calorimetry and X-ray diffraction measurements. Furthermore, electrical functionalities were also investigated by using the AC and DC electrical measurement units.

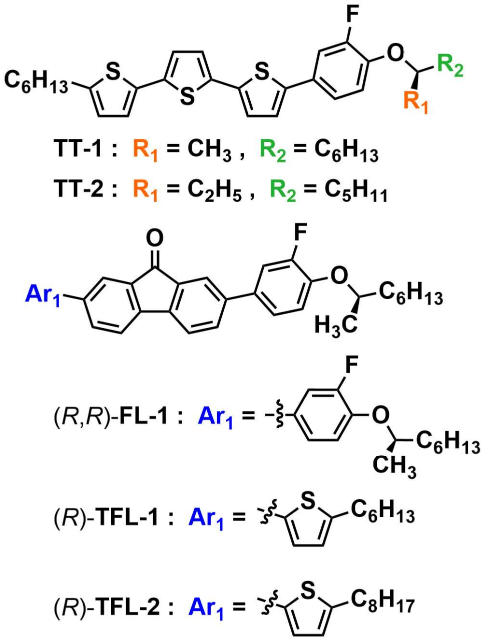

Figure 1: Chemical structures of chiral liquid crystalline π-conjugated compounds.

All these compounds of **TT-1**, **TT-2**, (*R*,*R*)-**FL-1**, (*R*)-**TFL-1** and (*R*)-**TFL-2** displayed polar smectic phases. The dielectric polarization hysteresis behaviors were observed by Sawyer-Tower method for the five compounds in their chiral smectic C phases. The carrier mobilities of each compound in the liquid crystalline phases were estimated to be on the order of $10^{-5}-10^{-3}$ cm^2 V^{-1} s^{-1} by the time-of-flight method. The specifics including the characteristics of BPVE will be discussed on the day.

Acknowledgements: This study was financially supported by a research grants from the Amano Institute of Technology and the Japan Keirin Autorace foundation in Japan.

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A5

Hydrogen-bonded systems

Engineering Hydrogen Bonding in LC Star-Shaped Triazines: Semiconductivity, Chirality and Supramolecular Memory Effect

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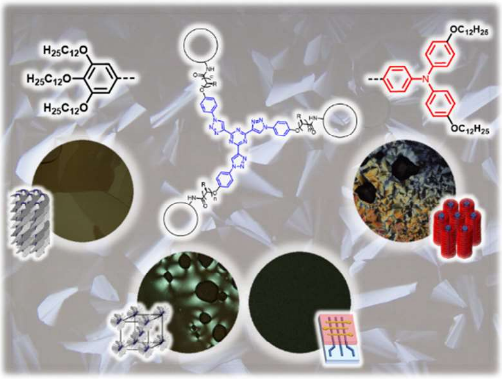
Keywords: columnar liquid crystals, cubic phases, hydrogen bonds, chirality, charge transport.

Liquid crystals (LCs) are an important class of soft nanostructured materials in which the molecular shape determines the molecular organization and hence their final properties.[1] C_3-symmetric star-shaped mesogens are versatile building blocks that can assemble into different types of mesophases.[2] Their tunable molecular design affords high control of the phase architecture since the nature of the core, the arms and the spacer between both parts can modify the intermolecular interactions that dictates the self-assembly process.



In this work we present two families of star-shaped tricarboxamides with C_3-symmetry that have flexible amide spacers linking a tris(triazolyl)triazine core to trialkoxyphenyl or triphenylamine (TPA) promesogenic units.[3] The presence of amide groups allows the formation of intermolecular hydrogen bonds that reinforce π-stacking and van der Waals interactions, promoting LC behavior across a wide temperature range. For 3,4,5-trialkoxyphenyl derivatives, the flexibility of the spacer promotes the formation of Col_h mesophases at room temperature, and cubic micellar mesophases (BCC) at high temperatures mediated by the fragmentation of columns with a supramolecular orientational memory effect. In the case of TPA derivatives, a reduced number of peripheral alkoxy chains leads to the formation of columnar mesophases throughout the full mesomorphic temperature range. Furthermore, the introduction of functional TPA units endows semiconducting properties to the material, resulting in high hole mobility values (10^{-2}-10^{-3} $cm^2\ V^{-1}\ s^{-1}$). In addition, the presence of a stereogenic center in the flexible amide spacer leads to macroscopic chirality.

Acknowledgements: This work was financially supported by the Spanish projects PID2021-122882NB-I00, PID2021-126132NB-I00 MCIN/ AEI /10.13039/501100011033/ and by "ERDF A way of making Europe", the Gobierno de Aragón-FSE (E47_23R- research group).

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Experimental and computational studies on non-symmetrical benzimidazole-based liquid crystals

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Keywords: Liquid crystal; Beinzimidazole; Self-assembly; Hydrogen bonding.

The development of self-assembled molecular systems is essential to the advances in the soft materials´ field.[1] Benzimidazole derivatives are extensively employed in many areas, including mesogenic materials.[2] In this work, we report experimental and computational results obtained for mesogenic behavior of amphoteric H-donor/accepting benzimidazole derivatives. The compound 2-(4-dodecyloxy-phenyl)1*H*-benzimidazole (1a) presents a stable enantiotropic phase from 85 to 177 ºC on cooling. POM analysis showed dendritc growth aggreagtes on cooling from isotropic liquid, which is consistent to SmB mesophase, and at lower temperature, an unidentified SmX texture is also observed (Fig. 1a and Fig. 1b). DSC analysis are in agreement to the POM findings. On cooling, phase transition was observed at 177 ºC and 154 ºC, for entering SmB and SmX phases, respectively. The existence of crystal phase was observed at 85 ºC, and a further crystal to crystal transition is visualized at 64 ºC. Computational study for tetramer-based supramolecular assembly of compound 1a have suggest that combination of hydrogen-bonding and hydrophobic interactions lead to a non-planar lamellar ("roof"-type architecture) organization (Fig. 1c), which is coherent to the smectic polymorphism observed for this compound. On the other hand, π-stacking interaction was not observed in this molecular model. At this moment, the effect of shorter alkyl chains as well as the effect of a second alkoxy group at the benzimidazole nucleus are been investigated aiming to fully comprehend the effect of the supramolecular interactions on packing and liquid crystalline behavior of these benzidazole-based soft materials.

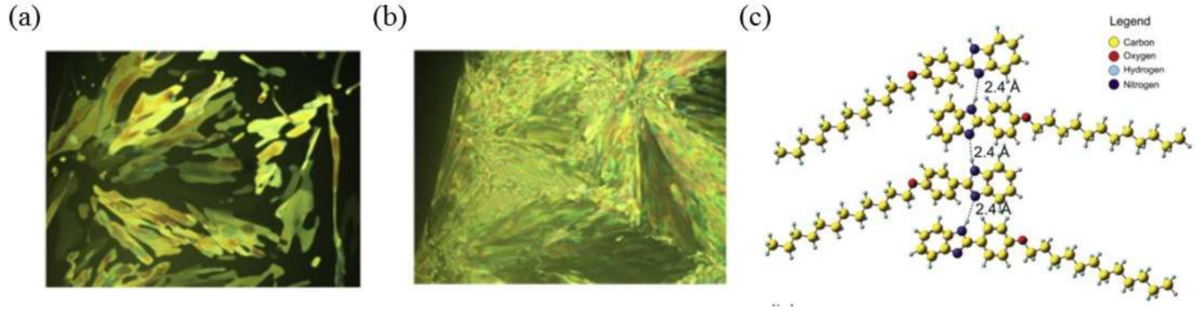

Figure 1: POM microphotographs of compound **1a** on cooling: a) at 176 ºC entering the SmB phase, and: b) at 101 ºC in the SmX phase; c) Side-view of the proposed computational model for self-assembly of **1a** obtained using the RM1 method and MOPACC2016 program.

Acknowledgements: CAPES, CNPq, Finep, FAPERN, Central of Analysis/IQ-UFRN.

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Fine-Tuning Functional Columnar Assemblies: Harnessing Hydrogen Bonding

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Keywords: columnar liquid crystals, hydrogen bonds, chirality, charge transport,

The implementation of functional materials through the exploitation of liquid crystal organizations relies on the efficient transfer of intrinsic molecular properties to the macroscopic supramolecular architecture. This transfer is strongly influenced by a precise molecular design, which exerts a pivotal role in the organization of molecules. In this framework, the inclusion of hydrogen-donor and/or hydrogen-acceptor molecular building blocks enables the utilization of hydrogen bonding interactions. As dynamic and directional non-covalent interactions, hydrogen bonds prove to be ideal for regulating interactions between molecules, thereby facilitating the targeted addressing and fine-tuning of their organization.[1]

This presentation concentrates on our latest progress in the development of highly organized functional columnar liquid crystals. These columnar architectures are realized through an assembly process utilizing (self-)complementary molecules, with the collaborative contribution of H-bonding and π-stacking. In our approach, we leverage hydrogen bonding to either reinforce π-stacking[2] or construct innovative supramolecular mesogens from simple molecular units.[3] The primary objective is the development of novel functional materials, with specific focus on properties such as the control of supramolecular chirality and charge transport.

Acknowledgements: This work was financially supported by the Spanish projects PID2021-122882NB-I00, PID2021-126132NB-I00 MCIN/ AEI /10.13039/501100011033/ and by "ERDF A way of making Europe", the Gobierno de Aragón-FSE (E47_23R- research group).

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A6

Photosensitive liquid crystals

A compact SiPM-based neutron Time-of-Flight detector using EJ-309

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Keywords: pulse shape discrimination, silicon photomultiplier, liquid scintillator, neutron Time-of-Flight

Organic scintillators with low Z-number materials are typically used to detect fast neutrons in mixed fields [1]. To distinguish neutrons and gamma-rays, a process called pulse shape discrimination (PSD) is necessary, which utilizes the difference in decay time between neutrons and gamma-rays in an organic scintillator [2]. The distribution of neutrons and gamma-rays after going through pulse shape discrimination tends to follow a two-Gaussian shape. Among several organic scintillators, liquid scintillators are widely used for PSD. Meanwhile, a silicon photomultiplier (SiPM) is a promising photosensor that could replace a conventional photomultiplier tube (PMT) in radiation detection. An SiPM has several advantages over a PMT, including compactness, cost-effectiveness, insensitivity to magnetic fields and power requirement. Our study attempts to investigate the pulse shape discrimination ability of liquid scintillator and verify the results with the neutron energy spectrum obtained with the neutron Time-of-Flight experiment. Furthermore, we would consider parameters that could contribute to the operation of SiPMs and see whether it affects the neutron Time-of-Flight results as well. In this study, EJ-309 will be used as the liquid scintillator, along with charge comparison method [3].

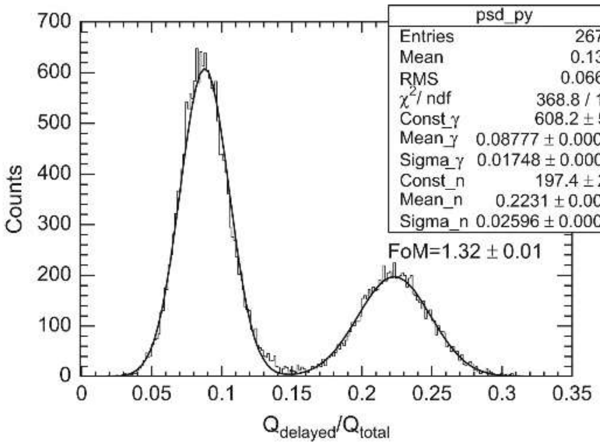

Figure 1: Example of neutron/gamma-ray PSD with EJ-309 liquid scintillator [4].

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Benzyloxy-terminated Isoxazole Liquid Crystals

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Keywords: isoxazole, semiperfluoroalkyl chain, smectic mesophase, benzyloxy-terminated

The synthesis and characterization of two benzyloxy-terminated isoxazole liquid crystals (ILCs) are described. The synthesis of the isoxazole ring was based on two steps: (3+2) 1,3-dipolar cycloaddition to furnish the isoxazoline cycloadduct and the subsequent MnO_2-oxidation. The liquid crystal (LC) behavior was accomplished by polarized optical microscopy (POM) and differential scanning calorimetry (DSC).[1] Flexible groups in ILCs allow molecular reorientation, leading to changes in mesophase behavior, affecting the stability and range of mesophases. Understanding the significance of these groups on the structure-property relationship is essential for designing advanced liquid crystal materials for a wide range of technological applications.

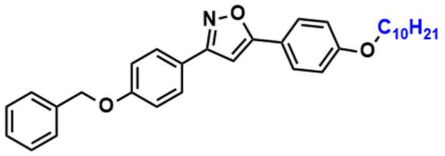
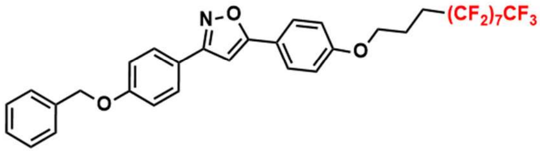
Alkyl chain  	Semiperfluoroalkyl chain 
Cr 133 SmC 148 SmA 162 N_{cyb} 169 I	Cr 161 SmA 279 I

Figure 1: Structures of the new 3,5-diarylisoxazoles with their transition temperatures (°C).

The presence of semiperfluorinated alkyl chains leads to organizational properties driven by microphase separation and steric effects.[2] These segments are not strongly miscible with aromatic and aliphatic segments and tend to be microsegregated from both,[3] which favors the appearance of structured materials in terms of layering and columns developments. Perfluorinated segments, characterized by high molecular volume, large surface area, and reduced flexibility compared to linear alkyl chains, influence molecular organization by affecting interfacial energy.[4] In the hydrogenated ILCs, cybotactic clusters were observed in the nematic phase (Ncyb), while the SmA and SmC mesophases showed monolayer and bilayer arrangements. As anticipated, replacement of the alkyl chain with a semiperfluorinated chain promoted the SmA mesophase and significantly impacted the mesophase range compared to the alkyl chain-containing ILCs, as seen in Fig. 1.

Acknowledgements: We are grateful to CNPq Ed. Universal 403.134/2021-8, CNPq/PQII 311195/2023-7, Ed. Fapergs/PqG n. 21/2551-0002121-7 and Ed. Fapergs/CNPq 07/2022 n. 23/2551-0000114-4 for the financial support.

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Illuminating mesophases: Isoxazolines with carbazole moiety

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Keywords: isoxazolines, dihydro-isoxazoles, 1,3-dipolar cycloaddition, carbazole

Exploring the dynamic optical landscape in materials science, fluorescent molecules with liquid crystal properties offer a gateway to diverse possibilities. Specifically, five-membered heterocycles like isoxazolines have been studied for their potential in design compounds with liquid crystal characteristics [1]. Leveraging the appeal of incorporating natural products into advanced materials, this work strategically aimed to synthesize isoxazolines with both liquid crystalline and fluorescent properties. The synthesis methodology involved the insertion of the fluorescent scaffold carbazole and utilization of natural products as key starting materials, thereby combining the advantages of both innovative design and sustainable resourcing. A series of 3,5-dissubstituted isoxazolines bearing a carbazole core at 5-position (Fig. 1A) were obtained through the 1,3-dipolar cycloaddition between nitrile oxides and 9-vinyl-carbazole. The nitrile oxides were generated *in situ* by the oxidation of oximes using sodium hypochlorite. Aromatic aldehydes (benzaldehyde, 4-nitrobenzaldehyde, 4-chlorobenzaldehyde, 4-bromobenzaldehyde, 2-methoxybenzaldehyde), *trans*-cinnamaldehyde (from natural sources), and extended arylethynylbenzaldehyde previously synthetized [2] were reacted with hydroxylamine for oxime synthesis. The cycloadducts were obtained with moderate to good yields and were purified by recrystallization in ethanol or acetonitrile. Preliminary fluorescent results from fresh solutions of **1g** and **1h** exhibited medium to high fluorescent properties when excited by ultraviolet radiation at 365 nm. A detailed fluorescence study is in progress. Furthermore, isoxazoline **1h** displayed monotropic liquid crystalline behavior upon cooling with a nematic mesophase, ranging from 170 ºC to 158 ºC, as depicted in Fig. 1B. The isoxazoline series reported here is an opportunity to analyze the fluorescence properties based on the size and the nature of aryl group installed at C-3 carbon atom of isoxazoline ring.

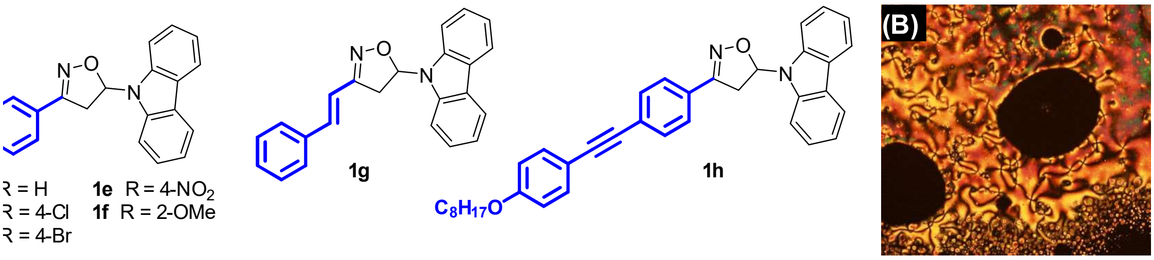

Figure 1: Isoxazolines with carbazole at C-5, highlighting the group at C-3 (A), and the observed nematic mesophase under polarized optical microscopy at 156 ºC for compound **1h**.

Acknowledgements: We are grateful to CNPq and FAPERGS ed. 07/2021 n. 21/2551-0002121-7; 07/2022 n. 23/2551-0000114-4 and 14/2022 n. 23/2551-0000919-6 for the financial support. I.L.G. thanks to CNPq/FAPERGS for his fellowship.

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Light-controlled refractivity modulation in azo-dye-doped liquid crystals

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Keywords: liquid crystal, nonlinear optics, refractive index, order parameter

Large birefringence and easy responsiveness to external factors have for long substantiated the almost ubiquitous presence of liquid crystals (LC) in various systems for light manipulation. The mechanism of the LC director reorientation has been widely employed in a great many of nonlinear optical effects despite rather long characteristic times and essential nonlocality. On the other hand, light-induced changes of the LC order parameter cause a fast and purely local nonlinear optical response fundamentally important as far as holography applications are concerned.

The light-excited molecule sitting in an LC medium interacts first with its closest neighbors, greatly affecting the orientational ordering of the latter. A phenomenological model of light-induced order modification (LIOM) accounts for the changes in LC optical characteristics due to light-stimulated modulation of the LC order parameter [1] and was employed to explain large observed optical nonlinearities with extremely fast as for a LC system recording times [2]. Then the modulations of the LC refractive index are determined as: $\delta n_{o,e} = -g\alpha\Delta n_0 C_{ph}$ ($n_{o,e}$ is the ordinary (extraordinary) refractive index with $g = -\frac{1}{3}\left(\frac{2}{3}\right)$, respectively, Δn_0 is the initial LC birefringence, C_{ph} is the concentration of light-excited molecules and α is a measure of the LC order parameter modification).

The light-induced changes of refractive indices of azo-dye-doped LC mixtures (the standard E7 and the dedicated highly birefringent, sexiphenyl's derivative doped mixture 2091D - possessing large birefringence up to 0.6 at 360 nm) were evaluated by measuring the diffraction efficiency of dynamic grating recording by means of two-wave mixing technique. Furthermore, the quantitative phase imaging by digital holography microscopy (DHM) [3] has been used as a comparative characterization procedure revealing good agreement.

The LIOM-type mechanism does not depend on the cell thickness, works for the whole range of light wavelengths and could be useful for fast control of optical signals of very high intensity, for instance, in the IR and well beyond.

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Liquid Crystals and Fluorescent Properties of Molecular Hybrid *trans*-Stilbene/Isoxazole.

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Keywords: Isoxazoles, *trans*-stilbene, hybrid materials, Smectic A mesophase, fluorescence

In this communication, we report the initial results of synthesis and characterization of molecular hybrid materials containing an anisotropic isoxazole segment and another bulky and photosensitive-terminated segment derived from *trans*-stilbene.[1] The combination of molecular segments responsible for mesomorphic and photosensitive properties is an interesting alternative to produce molecular hybrid materials and their applicability in various commercial devices. The anisotropic segment was synthesized from a [3+2] cycloaddition reaction, producing the isoxazoline adduct, followed by oxidation to the corresponding isoxazole.[2] The flexible spacer with ten carbon atoms carries a reactive-terminated leaving group[3] was inserted to allow the installation of the photoresponsive segment derived from *trans*-stilbene.[4]
The synthesis of the *trans*-stilbene-isoxazole hybrid compound was accomplished through a convergent synthesis between the advanced intermediates derived from isoxazole[2,3] and the resveratrol derivative[4], yielding a yield of 65% yield. Hybrid material displayed SmA mesophase with the sequence of transitions mesophase: Cr 107 °C SmA I 128 °C. Solution in DMC solvent exhibited medium fluorescent blue when excited by ultraviolet radiation at 365 nm. DSC, X-ray and UV-vis/Fluorescence studies of the tittle compound are in progress to characterize the new molecular hybrid *trans*-stilbene/isoxazole as described in Fig. 1.

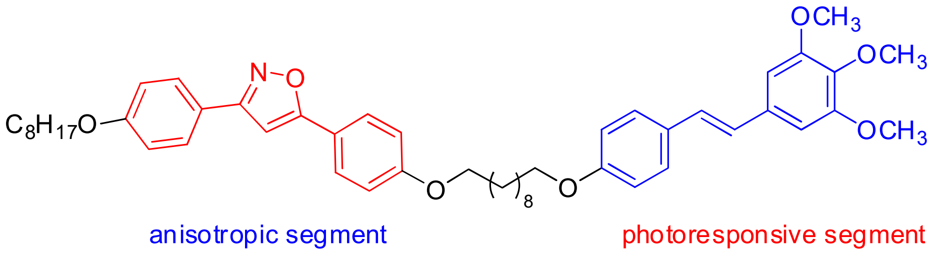

Figure 1: Hybrid *trans*-stilbene:isoxazole LC

Acknowledgements: We are grateful to CNPq and FAPERGS ed. 07/2021 n. 21/2551-0002121-7; 07/2022 n. 23/2551-0000114-4 for the financial support. A.A.M thanks to CNPq for his fellowship.

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Stimuli responsive achiral materials-transition from two to three-dimensional liquid crystal phases

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Keywords: Polycatenars, cubic phases, columnar phases, mirror-symmetry breaking

Alkyl chain engineering of liquid crystals (LCs) serves as an effective method for controlling self-assembly.[1] Designing stimuli-responsive multichain (polycatenar) LCs represents a promising strategy for developing functional materials. Herein, we present the design and synthesis of new π-conjugated polycatenar LCs incorporating azobenzene and oxadiazole units (Figure 1). The materials exhibit different types of LC phases ranging from three-dimensional 3D bicontinuous cubic (Cub$_{bi}$) to two dimensional 2D columnar phases depending on the length of the terminal chains. The Cub$_{bi}$ phases represent two different types, either the double gyroid type (Cub$_{bi}$/$Ia\bar{3}d$)[2] or the triple-network phase with $I23$ space group (Cub$_{bi}$/$I23$).[3] Chiral conglomerates were observed in the Cub$_{bi}$/$I23$ as well as in the liquid network phases exhibited by some homologues. Longer homologues form a hexagonal columnar LC phase, which could be aligned by cooling a molten sample under applied electric field. This alignment was attributed to dielectric polarization induced by the oxadiazole ring. Moreover, aromatic core fluorination was used as a successful tool to induce polarity in the columnar LC phases. Under UV irradiation, we were able to modify the LC phase structure via the reversible *trans-to-cis* photoisomerization of the azobenzene units. These findings could lead to potential applications of the reported materials in information-storage devices.

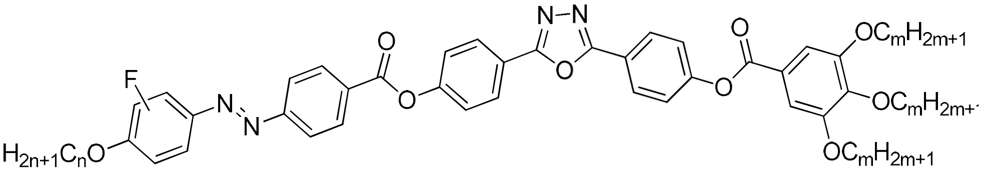

Figure 1. Chemical structure of the materials under discussion.

Acknowledgement: This work was funded by the German Research Foundation (DFG) (AL2378/1-2, 424355983).

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Substituted azobenzenes for photoactive LC systems

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Keywords: photosensitive, azobenzene, isomerization

The photo-manipulation of optical properties provided by the azobenzene molecular motif has shown great potential for future optical materials. Regardless if the driving mechanism of the photoactive soft material is photoinduced phase transition, photoalignment, or closely related photoactuation and photoinduced mechanical deformation, the azobenzene photoactive moiety still attracts much attention. Unfortunately, most studies are limited to simple liquid-crystalline azocompounds, commercial azo dyes or photoalignment agents, and thus there are no systematic data regarding the correlations between successfully varying the molecular characteristics of these materials and the photo-optical behavior of the resulting material. At the same time, majority of reported azobenzene materials used for liquid crystalline systems show poor kinetic stability of photogenerated Z isomer and very often a bad compatibility with the LC matrix when used as photosensitive dopants resulting in various degree of aggregation [1]. Here, we show our efforts to understand the chemical structure–property relationships of azobenzene photosensitive materials in liquid crystal systems. Through a synthetic study, we tried to help answer typical questions concerned with azobenzene photosensitive compounds. We focused specifically on the following three questions. How to increase the compatibility of the photosensitive azobenzene compounds with other components of the final liquid crystalline mixture? What is the molecular design of azobenzene derivatives with high/low kinetic stability of the photogenerated Z isomer and thus the high/low stability of the photoinduced changes of physical properties of the final material? How to design the materials effectively switchable by the desired wavelengths and thus to obtain effective photo-tuning of physical properties? The actual study was focused on substituents in *para* positions to -N=N- bond and the effects of lateral substituents on mesomorphism, photochemical and thermal isomerization as well as absorption properties in the UV-Vis region.

Successful application of the substituent trends will be demonstated on several examples of photosensitive liquid crystalline systems [2,3].

Acknowledgements: This work is funded by the Czech Science Foundation (Project No. 22-16499S and 23-42944L).

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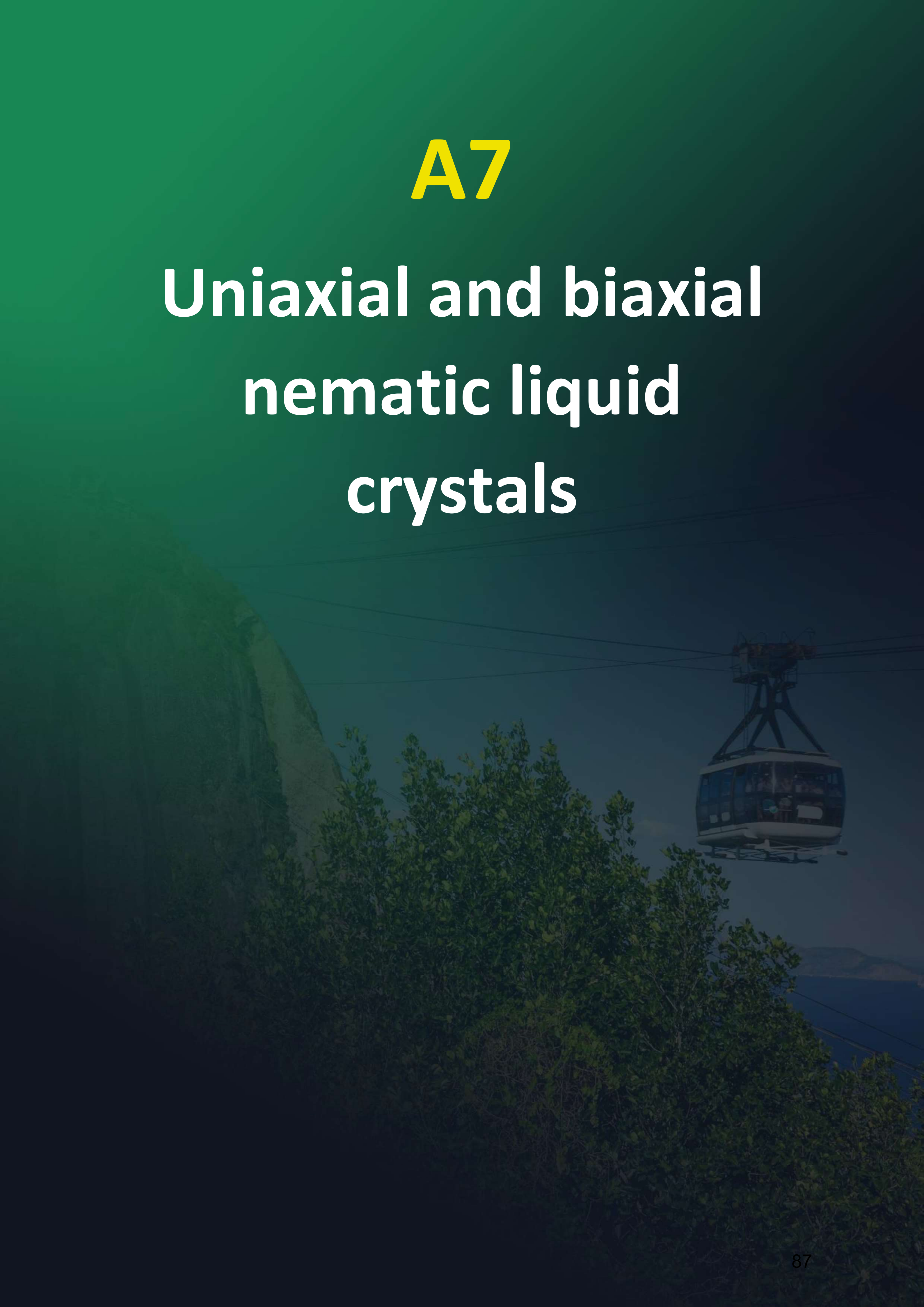

A7

Uniaxial and biaxial nematic liquid crystals

Elastic and Inelastic X-ray Scattering: Understanding the Structures and Dynamics of Nematic and Smectic Liquid Crystals

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Keywords: Elastic, Inelastic X-ray Scattering, Nematic, Smectic, Structure, Dynamics

X-ray scattering methods have played a pivotal role in understanding the structures and dynamical properties of liquid crystal phases from the beginning of the field. In the early stages, non-monochromatic X-rays and inefficient detectors, such as ionization gauges, were used. Quite remarkably, researchers could distinguish the structure of the nematic (N) phase from that of the isotropic state in octyl alcohols [1], estimate the intermolecular separation along their long and short axes, and the size of molecular aggregates in these phases with good accuracy.

High-resolution methods, developed with the advancements in the generation and detection of X-rays and new ways to prepare well-collimated monochromatic beams, enabled tests of fundamental scientific concepts such as Landau Peierls instability in the smectic-A (SmA) phase, universality of the N-SmA phase transition, 2-D melting, and bond-orientational order in hexatic phases. Synchrotron-based experiments further enabled measurements of the first ($<P_2(\theta)>$), second ($<P_4(\theta)>$), and third order ($<P_6(\theta)>$) order parameters, heliconical tilt angle, and molecular distribution functions to differentiate between various phases including the N, twist-bend N phases of CB7CB, and the de Vries SmA and SmC phases of siloxanated mesogens and test theoretical models.

Very recently, the inelastic x-ray scattering (IXS) beamline 10-ID at the National Synchrotron Light Source II, with an energy resolution of about 2 meV, has opened the door to investigations of phononic collective excitations in LCs. The IXD beamline was used to investigate the isotropic, N, and SmA phases of D7AOB and 5CB LCs. The results show the coexistence of transverse and longitudinal phononic modes, a characteristic response of solid materials, and a strong mixing of phonon modes arising from in-phase and out-of-phase movements. The *phononic* response of the three phases is very different: the SmA phase reveals longitudinal (LA) and transverse acoustic (TA) and optical modes. In contrast, the isotropic and N phases exhibit only the LA and TA modes. The LC systems are suitable for further IXS investigations of the propagation of sound and heat and for understanding their unique optomechanical and nanoacoustic properties. X-ray experiments on LCs over the past ~100 years will be discussed.

Acknowledgements: Supported by the National Science Foundations and US Dept of Energy.

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Experimental Conditions for the Stabilization of the Lyotropic Biaxial Nematic Mesophase

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Keywords: lyotropic, nematic, structure, laser conoscopy

Nematic is one of the most common phases among the lyotropic liquid crystalline structures. They have been widely investigated during last decades. In early studies, two uniaxial nematic phases (discotic, N_D, and calamitic, N_C) were identified. After the discovery of the third one, named biaxial nematic phase (N_B) in 1980, some controversies on the stability of biaxial nematic phases began and still continue in the literature. From the theoretical point of view, the existence of a biaxial nematic phase is well established. From the experimental point of view, considering a mixture surfactant/co-surfactant/solvent, the relative alkyl chain length of both surfactant, m, and co-surfactant (e.g., an alcohol), n, the higher (smaller) the value of the m (n), when compared with the value of n (m), the larger the phase domains of the N_D and N_B (N_C). Indeed, this situation is a result of the molecular segregation of the surfactant and alcohol molecules in the micelles. In the case of the specific interactions between head groups of the surfactants and the counterions/ions of strong electrolytes present in the mixture, in terms of their kosmotropic and chaotropic characters, choosing the surfactant and the electrolyte with slightly opposite (strongly same) character may help to stabilize a lyotropic mixture of the N_B (N_D) phase. Strongly opposite characters of both ionic species, head groups and the ions present in the mixture, stabilizes the N_C phase. This communication aims to bring information about the historical development of the nematic phases and summarize the recent studies on how to stabilize different nematic phases from the experimental conditions, choosing the suitable constituents of lyotropic mixtures to get the biaxial nematic phase.

Acknowledgements: CNPq - (465259/2014-6); FAPESP - (2014/50983-3; 2016/24531-3); CAPES; INCT-FCx.

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High Molecular Biaxiality of Nematogens and the Impact on Materials Properties

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Keywords: Biaxial nematogens, Structure-Property relationship, Molecular Dynamics, X-ray, X-ray simulation, charge carrier mobility,

"Biaxial nematic liquid crystals: fact or fiction?" was the title of a review at the beginning of the second intense research period to find the holy grail of LC science.[1] 13 years later, after an immense effort, especially in the area of bent-shaped molecules, no low-molar weight material has been convincingly approved for its phase biaxiality.[2] This keynote will give a short overview on the historical background and the challenges to be overcome either on molecular design or alignment of the secondary director. Although, the latter is confirmed macroscopically in the range of hundreds of nanometers to a few micrometers, a permanent uniform alignment large enough to be visualized by Conoscopy or X-ray scattering remains difficult. Eventually, a new class of roof-shaped nematogens (Figure) will be presented, for which molecular biaxiality approach an optimum. Biaxial clusters have been shown to exist by XRS and NMR relaxometry.[3] Recently, MD simulations combined with X-ray simulations confirmed these findings for a lead structure **1a**.[4] High biaxiality parameters of up to B = 0.27 has been found in this mesogen family. Further evidence has been found by the record electron mobility revealed by the TOF technique for compound **1b**, which can be rationalized by the biaxial self-assembly of the mesogens in the nematic phase.

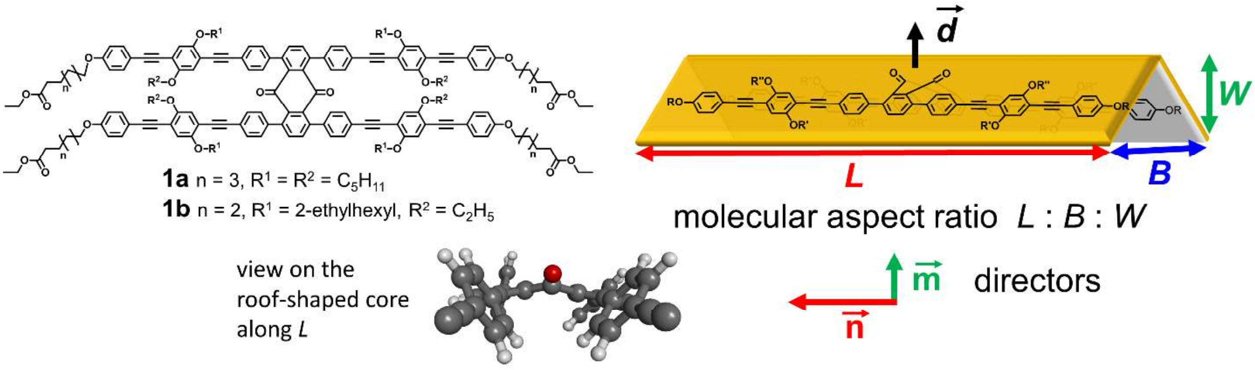

Figure. General structure of roof-shaped nematogens.

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Polarized Raman spectroscopy applied to lyotropic liquid crystal

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Keywords: Lyotropic liquid crystal, polarized Raman spectroscopy, phase transition

One of the most important phase diagrams of lyotropic nematic liquid crystals has been reported in the literature, in which two uniaxial (discotic – N_D and calamitic – N_C) and one biaxial nematic (N_B) phases were characterized [1]. The N_B phase appears to be an intermediate phase along the border between the two uniaxial nematic ones. Several techniques [2] have been used to observe phase transitions in lyotropic mixtures. For a concentration line in the Saupe diagram, whose $N_D – N_B – N_C$ transitions occur with increasing temperature, conoscopic images showed that inside the biaxial range, beyond the known biaxial positive (N_B^+) nematic phase, we also found a biaxial negative (N_B^-) nematic phase [3,4]. In this work, polarized Raman spectroscopy will be used to verify the phase transitions in a sample already known from the literature. This is a technique that probes vibrational modes associated with specific chemical groups, and therefore presents a detailed insight into the chemical composition of the sample and can provide information about the orientation of the molecules inside the micelles, allowing the determination of their orientation in the different phases of the liquid crystal. Figure 1 presents the angular variation of the Raman peaks intensity associated with the stretching modes of CH_2 and D_2O at different temperatures. Where a change in symmetry is clearly observed, indicating transitions with increasing temperature. Allowing for the difference between the maximum and minimum intensities (h) as a function of temperature (Fig. 1(c)), it is possible to identify the temperatures of the phase transitions.

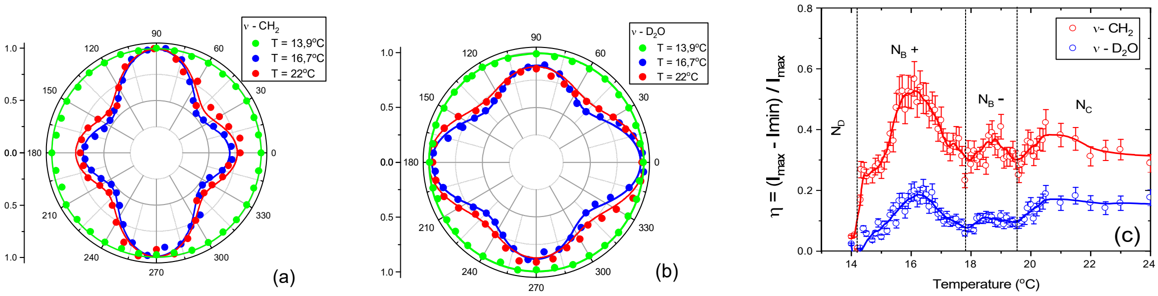

Figure 1: (a) and (b) the angular dependence of the intensities peaks associated with the stretching of the CH_2 and D_2O, respectively. (c) Parameter η as a function of temperature.

Acknowledgements: To FINEP, CNPq, INCT – FCx and Capes for the financial support of this work.

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Polarized Raman spectroscopy: Study of phase transition in thermotropic liquid crystal

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Keywords: Polarized Raman Spectroscopy, phase transition, 5CB, 8CB.

In their pioneering work, Jen *et al.*[1] laid the foundations for simultaneously identifying the first two nontrivial orientational order parameters, $\langle P_2 \rangle$ and $\langle P_4 \rangle$, in thermotropic liquid crystals using polarized Raman spectroscopy. In this technique, measurements of Raman depolarization ratios under different orthogonal linear polarization conditions are used to identify the order parameters. More recently, Zhong et al. [2] implemented a new sample rotation method, which was applied to a quartz crystal cut in the 'ac' crystallographic direction, demonstrating that the technique can be used in the study of anisotropic materials. The objective of this work is to verify whether this method can be applied to non-rigid systems such as samples of thermotropic liquid crystals (*5CB* and *8CB*), whose phases and transition temperatures are already well established in the literature [3]. Figure 1 presents the angular dependence of the Raman peaks intensity associated with the stretching mode of the $C \equiv N$ for the *8CB* sample at different temperatures. From the difference between the maximum and minimum intensities ($h = 1 - I_{min}/I_{max}$) as a function of temperature (Fig. 1(b)), the phase transition temperatures were determined, which are in agreement with the literature.

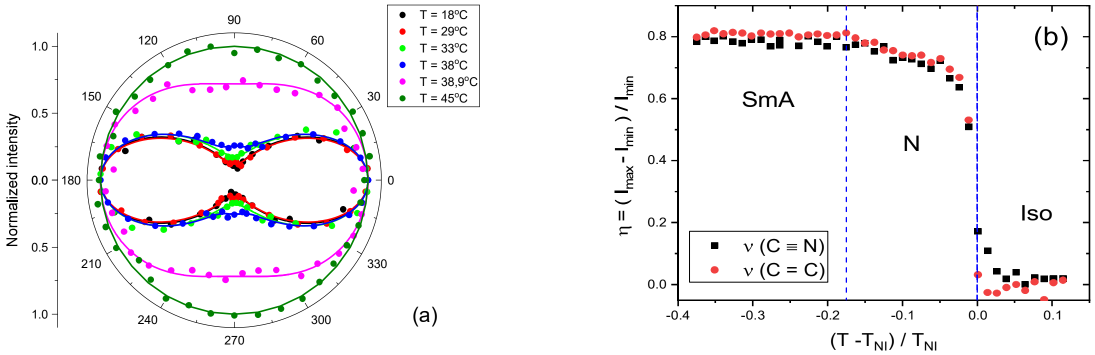

Figure 1: (a) Angular dependence of intensity to $\nu(C \equiv N)$ and (b) Parameter η as a function of reduced temperature to 8CB sample. T_{NI} is the nematic-isotropic transition temperature.

Acknowledgements: To FINEP, CNPq, INCT – FCx and Capes for the financial support of this work.

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The influence of the relative concentrations of the surfactant sodium dodecyl sulfate and co-surfactant decanol on the rheological behavior of uniaxial lyotropic lyomesophases

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Keywords: (Liquid Crystal, Lyotropic, Nematic, Rheology)

In this work we will study the rheological response of the nematic lyotropic system sodium dodecyl sulfate (SLS), decanol (DeOH), and water (H_2O) to changes in the relative concentration of the mixture constituents, expressed from the molar ratios $M_d = DeOH/SLS$ and $M_w = H_2O/SLS$ [01]. Calamitic nematic (N_C) solutions were obtained in line with the works of Thiele [02] and Amaral [03]. Initially, the molar ratios were decreased from $M_w = 46.69$ and $M_d = 0.374$ to $M_w = 40.63$ to $M_d = 0.338$, respectively; During this process the molar concentration of the DeOH cosurfactant was fixed at 0.315 mmol/g of sample. Subsequently, the Mw molar ratio decreased from 45.03 to 44.26, as the Md molar ratio increased from 0.293 to 0.383; In these mixtures the molar concentration of the SLS surfactant was fixed at 0.874 mmol/g of sample. We have made rotational and oscillatory rheological measurements. The results will be discussed in terms of the changes observed in important rheological parameters: viscosity, consistency index, fluidity index, elastic recovery modulus and viscous dissipation modulus.

Acknowledgements: From Brazil, the National Council for Scientific and Technological Development (CNPq – 465259/2014-6), the Coordination for the Improvement of Higher Education Personnel (CAPES), the National Institute of Science and Technology Complex Fluids (INCT-FCx), and the São Paulo Research Foundation (FAPESP – 2014/50983-3)

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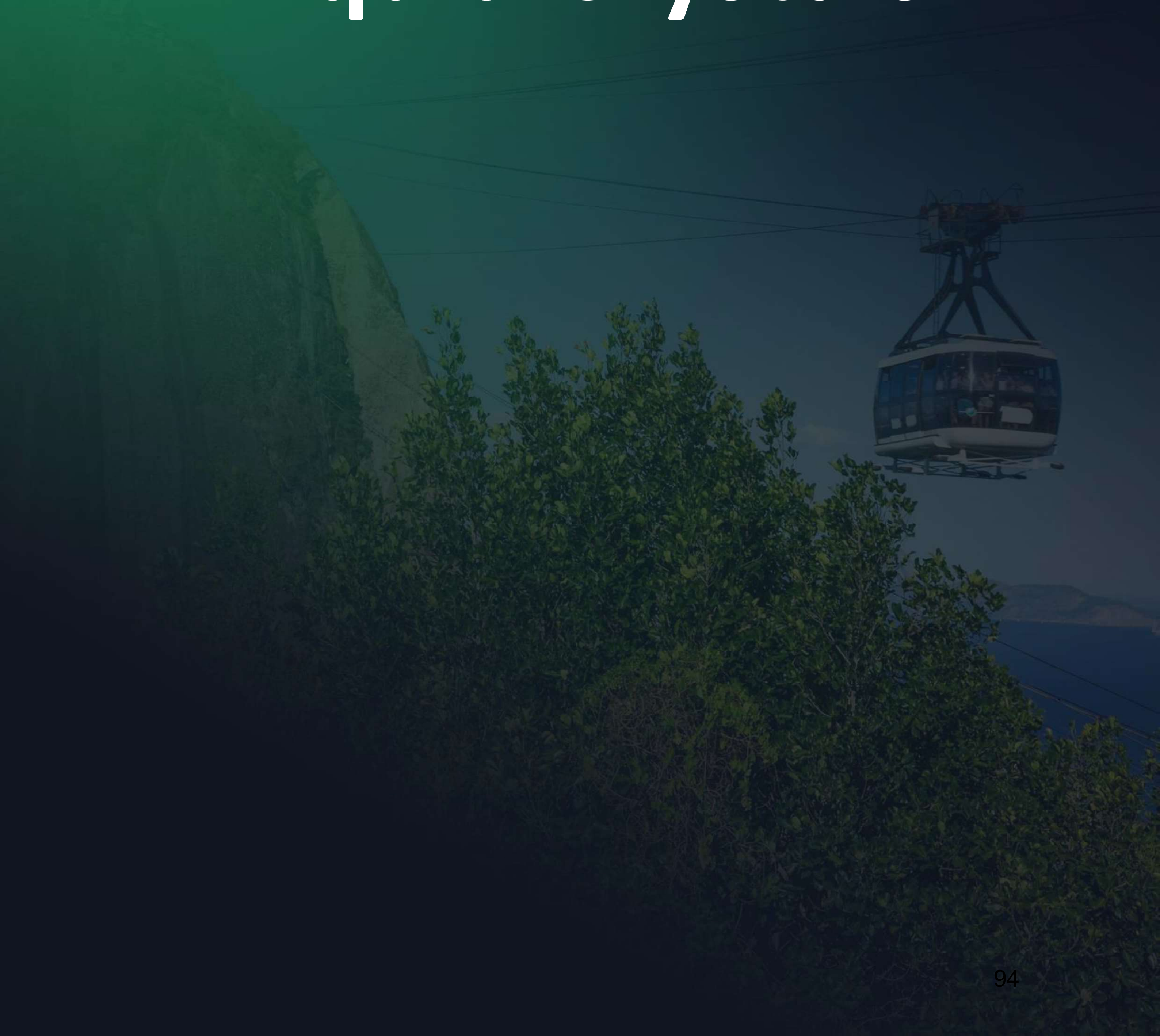
B

Macromolecular Liquid Crystals



B1

Polymers, elastomers and gels

Colorimetric Humidity-Sensing Liquid Crystal Elastomer Actuators

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Keywords: Liquid crystal elastomer, actuator, humidity sensing, stimuli-triggered motion, azobenzene

We report the synthesis, characterization and study of new liquid crystal elastomers (LCEs) for stimuli-controlled actuators capable of colorimetric humidity sensing. The designed LCE structures feature amino azobenzene moieties either as side groups or on the chain backbone, which can be protonated by an acid solution to render LCE actuators hygroscopic. When a protonated LCE actuator is in an environment of higher humidity, it absorbs more water and changes its color due to the deprotonation of azobenzene by water molecules, because the protonated and deprotonated azobenzene absorb visible light at different wavelengths. The initial color of the actuator and its sensitivity to humidity variation are determined by the extent of acid protonation on the LCE surface, and the reversible color change can be distinguished by the naked eye over a wide humidity range. This humidity-sensing LCE is used to fabricate cylindrical rod actuator that can autonomously roll on a hot surface while reporting the humidity change through its color change. Moreover, by applying water mist to selected area of a rolling rod actuator, the moisture can act as a stimulus to change or reverse the rolling direction and reduce the rolling speed. The achieved colorimetric humidity sensing capability endows LCE actuators with an intelligent function and can be explored for application.

Dynamic Pressure-Sensitive Adhesion from Liquid Crystal Elastomers

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Keywords: (liquid crystal, pressure-sensitive adhesion, polymers, gels, and elastomers)

liquid crystal elastomers (LCEs) exhibit unusually high vibration damping, which has been assumed to cause their anomalously strong pressure-sensitive adhesion (PSA).[1] Here we investigate the mechanism behind this enhanced PSA by preparing thin adhesive tapes with LCEs of varying chemical formulations, characterizing their material and surface properties, and examining their adhesion characteristics using a standard set of 90-degree peel, lap shear, and probe tack tests. Our findings confirm that the enhanced PSA is present only in the nematic phase of the elastomer, and that the strength of bonding takes more than 24 hours to reach its maximum value. This extended saturation time is due to the slow relaxation of local stress and director orientation in nematic domains after pressing against the surface. We demonstrate this mechanism by showing that a freshly pressed and annealed tape achieves the same maximum bonding strength upon cooling, when the returning nematic order is forming in its optimal configuration in the pressed film.

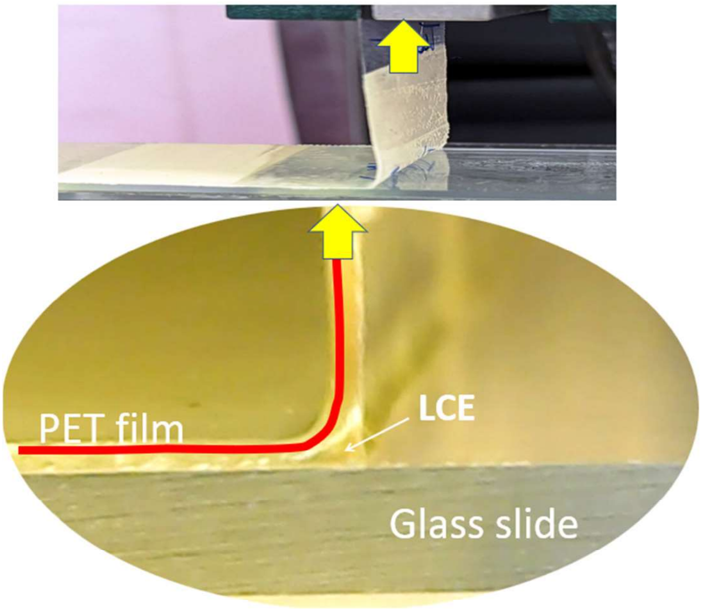

Figure 1: Peel testing of an LCE PSA adhesive

Acknowledgements: (This work was supported by the Royal Society via University Research Fellowships (URF\R1\221104)

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Electropolymerization Process as a New Tool to Obtain High Ordered Alignment Layers

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Keywords: Polymers, Methacrylic monomers, High ordered smectics

We are studying a new electropolymerization process with calamitic liquid crystals [1-4], which is carried out in the absence of solvents or added electrolytes. The process is achieved by applying a direct electric field to (meth)acrylic monomers in sandwich glass cells covered with ITO electrodes. The major advantage of this process is the ability to obtain highly oriented films of side chain liquid crystalline polymers (SC-LCP) when using planar aligned cells.

Based on a homologous series of 12 acrylates (A6En, with n=1-12) [2] we explore the occurrence of high order smectic phases after the polymerization process. The results shown that the so obtained PA6E4 polymer yielded a well aligned SmB phase at room temperature (Figure 1).

The polymerization of monomers was also performed by UV to compare both processes. Insight in the mechanism involved will be presented. Photoalignment and EP are two distinct processes, which can be synergically used to produce some liquid crystal devices for optoelectronics applications. The obtained data as well as the SAXS characterization will be presented.

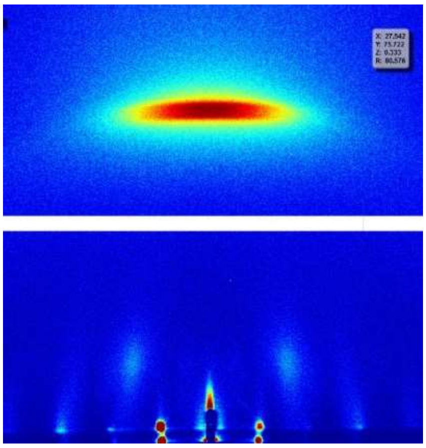

Figure 1: GIWAXS pattern of PA6E4 in the SmB phase

The new polymerization process is a powerful technique that can be synergistically employed in specific applications, especially in the development of advanced liquid crystal devices and optoelectronic systems. The precise implementation and potential benefits depend on the desired functionality of the final device.

Acknowledgements:

This work has been financed by Fondequip Mediano, EQM200266 and Anton Paar AFM Influencers Program

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Evaporation-induced self-assembly of Bio-LCs and its application

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Keywords: DNA, LC, evaporation-induced self-assembly, orientation control

Evaporation-induced self-assembly (EISA) is a process that has gained significant attention in recent years due to its fundamental science and potential applications in materials science and nanotechnology. This technique involves controlled drying of a solution or dispersion of materials, forming structures with specific shapes and sizes. In particular, liquid crystal (LC) biopolymers have emerged as promising candidates for EISA due to their highly ordered structures and biocompatible properties after deposition. This review provides an overview of recent progress in the EISA of LC biopolymers, including DNA, nanocellulose, viruses, and other biopolymers. The underlying self-assembly mechanisms, the effects of different processing conditions, and the potential applications of the resulting structures will be discussed.

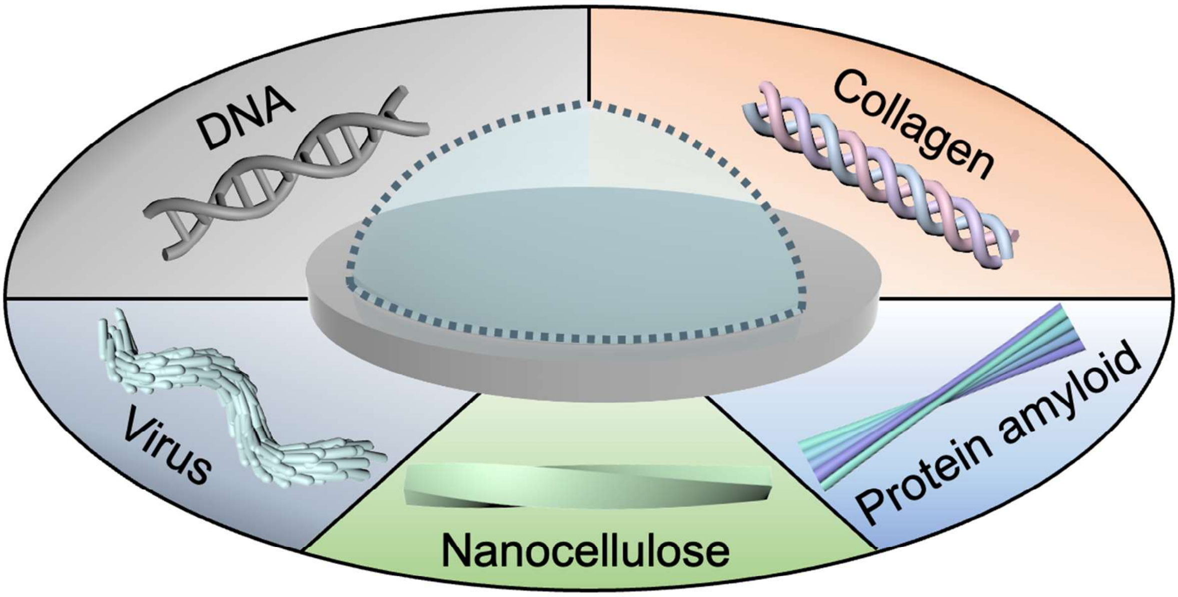

Figure 1: Evaporation-induced self-assembly of biomaterials

Acknowledgements: This was supported by a grant from the National Research Foundation (NRF) funded by the Korean Government (MSIT: 2021M3C1C3097646, 2018R1A5A1025208 and RS-2023-00273025).

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Halogen-bonded shape memory liquid crystal polymer

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Keywords: halogen bonding, shape memory, liquid crystal elastomer, stimuli-responsive materials, programming.

Stimuli-Responsive Liquid Crystalline Elastomers (LCEs) are a class of materials that can undergo significant changes in their properties and shape in response to external stimuli. In particular, harnessing the power of halogen bonding (XB), a non-covalent interaction between an electron-deficient halogen atom and a Lewis base, holds great potential for developing advanced LCEs with unique functionalities. In our study, we present a novel approach utilizing a liquid crystalline network comprising both permanent covalent crosslinks and dynamic halogen bond crosslinks. By incorporating XB into the LCE matrix, we achieve a reversible thermo-responsive shape memory behavior. The I···N halogen bond, a widely studied motif in crystal engineering, plays a pivotal role in enabling temporary shape fixation at room temperature and subsequent shape recovery when exposed to human body temperature. Notably, our research showcases the remarkable versatility of shape programming in these halogen-bonded LCE networks through simple human-hand operation. Additionally, we propose a micro-robotic injection model that allows for complex 1D to 3D shape morphing in aqueous media at 37 °C (**Figure 1**). Through meticulous structure-property-performance studies, we establish the indispensable contribution of the I···N crosslinks in driving the shape memory effect observed in our halogen-bonded LCEs. The introduction of halogen bonding expands the toolbox for designing smart supramolecular constructs with tailored mechanical properties and thermoresponsive behavior, opening up exciting possibilities for future medical devices and other advanced applications. [1,2]

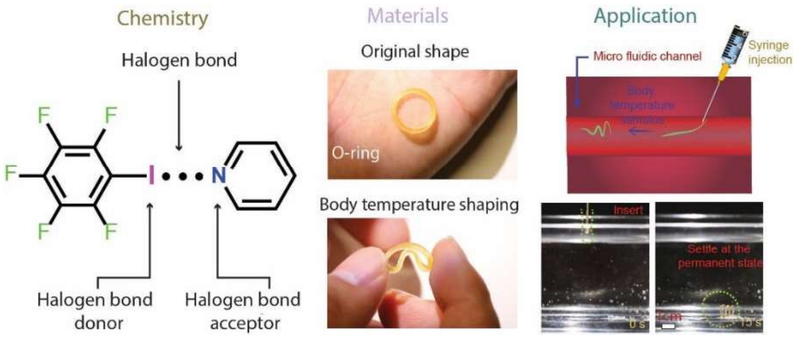

Figure 1: Halogen-bonded shape memory liquid crystal polymer.

Acknowledgements: Academy of Finland, European Research Council and Academy Postdoctoral Researcher projects.

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Understanding the impacts of LCE formulation on actuation and alignment

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Keywords: liquid crystal, elastomers, actuation, formulation, additive manufacturing,

Liquid crystal elastomers (LCEs) reversibly change shape when exposed to local external stimuli, chemical, electrical, mechanical and/or thermal in origin. Recently, our colleagues have demonstrated that direct ink written elastomers carrying gold nanorods could respond locally to light and globally to heat gradients, their shape shown to be modulated using a laser rastering across the sample to demonstrate the former [1]. However, in addition to non-polymer additives impacting controlled actuation in LCEs, additives such EDDET, n-butylamine and 5CB co□formulated with differing ratios of RM82, RM257 and other benzene-acrylate type monomers can affect whether films produced from them are amenable to photochemical and mechanical alignment, and, crucially, whether there can be significantly repeatable actuation from these films. As we see, successful alignment is not always indicative of a film's ability to actuate. This becomes even more apparent when LCE resin mixtures prone to side chain polymerization do not benefit from the addition of additives or spacers due to their chemistry as well. Here, we present an investigation of the properties of both side chain & main chain elastomer mixtures produced with additives, as well as the extent to which these formulations can be actuated. An understanding of actuation in 1-layer films will inform how DLP (digital light printing) and magnetic alignment printing processes can be adapted to accommodate multiple layer film printing with precise director alignment control.

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Prepared by LLNL under Contract DE-AC52-07NA27344. Release # 1092178

Liquid Crystalline Elastomers Prepared Via Thiol-ene Chemistry

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Keywords: Liquid Crystal Elastomer, Cholesteric, Polymer Chemistry, Optics, Stimuli-Response

Liquid crystalline elastomers (LCEs) are lightly crosslinked elastomers with unique anisotropic properties. They are increasingly considered for functional use in automotive, aerospace, robotics, and biological applications. LCEs that retain the cholesteric phase (CLCEs) are optical materials that self-organize into a helicoidal structure. The rotation and periodicity of the refractive index across the thickness of the material forms a 1-D photonic bandgap resulting in a reflection notch in the UV to MWIR and beyond. Our focus is on optimizing the chemistry to make transmissive CLCEs with homogeneous properties, tunable crosslink density, and low haze. Thiol-ene photopolymerization is a one-step click chemistry that yields homogeneous polymers with controllable crosslink density.[1] Here, we detail the use of thiol-ene reactions to make LCEs and CLCEs amenable to surface alignment. The stimuli-responsive behavior of optical CLCEs was explored which can be applied to applications such as ophthalmic devices or window coatings for the built environment.

Acknowledgements: This work was funded by the Department of Defense through the National Defense Science and Engineering Graduate Fellowship Program.

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Liquid crystalline microstructures with spatially controlled anisotropy

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Keywords: direct laser writing, liquid crystal polymers, director orientation

Many of the most interesting properties of cross-linked liquid crystals arise from director orientation, which can be tailored for specific applications through methods ranging from mechanical stretching, rubbing, electric and magnetic field, or photopatterning. When these methods are used in conjunction with direct laser writing (DWL), microstructures of desired geometry and reversible shape change can be created.

In our research, we focus on developing a methods that would enable layer-by-layer changes in director orientation during the DWL process to manufacture structures capable of complex deformation in response to external stimuli. We found out that this can be achieved by programming the direction of laser scanning during the process of 2-photon polymerization, as the alignment of subsequent lines affects the neighboring molecules. The effect is clearly visible when cross-linked LC microstructures are printed on a bare substrate (Fig. 1A). This method can yield birefringent structures on surfaces with complex geometry that cannot be easily modified by other techniques e.g. the end-face of an optical fiber.

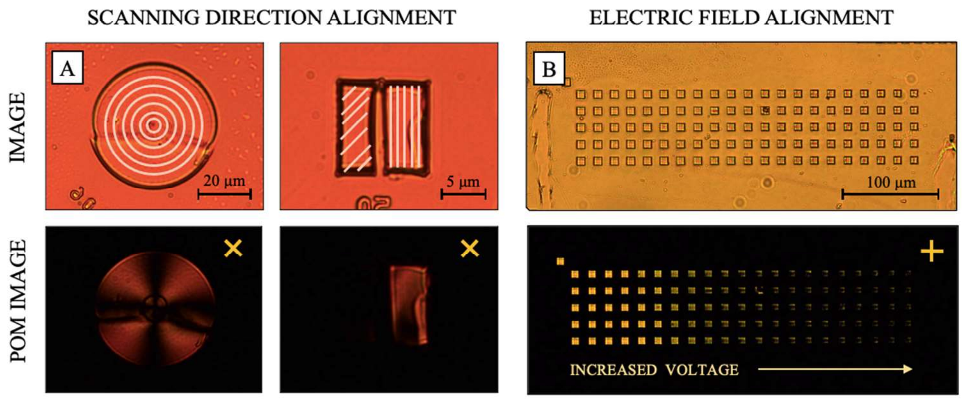

Figure 1: Microscope images of (A) LC network and (B) LC gel microstructures printed using described alignment techniques. In (A) laser scanning direction has been marked.

The other method employed for dynamic director change involves electric-field alignment, observed in liquid crystal gels with mesogens with high dielectric anisotropy. Our research has demonstrated that structures with varied director orientation can be produced adjacently through adjustments in the voltage applied to the LC cells during laser printing (Fig. 1B).

Acknowledgements: This work was funded by the Polish Ministry of Science and Higher Education under the Pearls of Science program. The authors thank W. Piecek, P. Morawiak and R.Węgowski from the Military University of Technology in Warsaw for their assistance.

Polymer Stabilization of Nematic Liquid Crystal Confined in Stripes

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Keywords: Nematic; Confinement; Polymer-stabilization; Stability; Sensors

Chemically patterned stripes of varying aspect ratios were fabricated on glass surfaces. A hydrophobic surfactant surrounding the stripes allowed confinement of a nematic liquid crystal mixture (NLC) containing ≤5wt% of RM82 reactive mesogen and a drop of MBF UV photoinitator. The top NLC stripe surface is open to air, and the lower surface is either glass or a rubbed polymer alignment layer. The former contrasts with the literature where the majority of NLC polymer stabilization occurs within a cell[1]. It has been shown in the literature that NLC polymer stabilization can describe director fields in a cell[2]. For the geometry in this work, the commonly seen central defect of the confined stripe can be faithfully reproduced after UV curing and NLC removal, with shrinkage of the system also observed after NLC removal.

Factors relating to texture stability are also discussed. For example, it was found that the system with no RM82/MBF had a significantly different texture under polarized optical microscopy than the UV cured RM82/MBF mixture. The texture was different after the UV cured system was annealed (Figure 1). A nematic-isotropic temperature close to the expected value was measured for the UV-cured system during annealing, demonstrating the thermal stability of NLC properties. Polymer stabilized NLC have been demonstrated in the literature to detect analytes e.g toluene[3]. The free-surface geometry in this work allows a large surface area for this. An understanding of the stability can be used to develop longer-lasting chemical sensors.

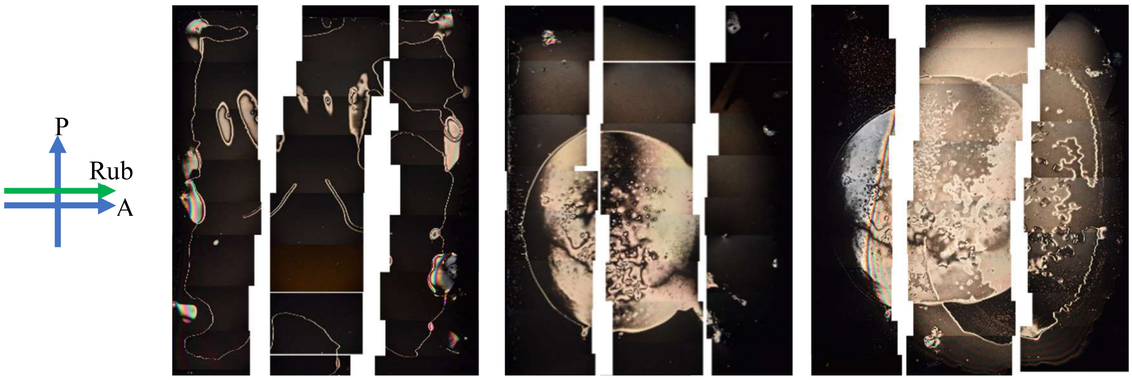

Figure 1- Demonstrative composite transmission polarized optical microscopy images of 8.8±0.1µL NLC confined in a ***20x16mm*** *rectangle with* (left) *no RM82/MBF,* (middle) *UV cured RM82/MBF, and* (right) *middle system annealed. The rubbing direction is approximately aligned with one of the crossed polarisers.*

Acknowledgements: *Funding:* EPSRC, UKRI.

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The relationship among elastic rheological behavior, network entanglement, and mesoscopic scales in: Solutions of giant micelles and biopolymer gels.

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Keywords: Worm-like micelles, mesoscopic scales, rheology, micro-rheology, biopolymer gels

The elastic contribution to the fluid dynamics of wormlike micellar solutions makes these fluids unique due to the distinctive self-assembled micellar network formed by cylindrical micelles. Measured mesoscopic scales of the micellar network related to the degree of entanglement can guide our understanding of the origin of elastic forces and their effect on rheological response. Different experiments were made to determine how elastic forces modify the rheological behavior in systems made of different ratios of hexadecyltrimethylammonium bromide (CTAB)/sodium salicylate (NaSal) and different ratios of CTAB/$NaNO_3$. Diffusive wave spectroscopy micro-rheology was performed to measure the mean square displacements of microspheres embedded in the micellar fluids to obtain their high-frequency viscoelastic spectra. With this information, the ratio of the total contour of the micelles to the entanglement length was estimated and correlated with the rheological behavior. This ratio was valuable information for understanding the origin of the contribution of the elastic forces from a molecular point of view on the fluid dynamics of wormlike micelle solutions.

The evolution of mesoscopic scales in biopolymer gelatin gels was also explored using micro-rheology. Depending on how they form, their linkings are commonly classified as physical, chemical, or hybrid. In hybrid gels, the physical and chemical crosslinking mechanisms run simultaneously. No matter the linking process, as time elapses after gelation starts, the persistence length of the unstructured, non-bonded flexible polymer sections decreases due to the formation of bonds. The time evolution of the gel network's mesh size roughly follows an exponential decay. In the hybrid case, the persistence length is not a mixture of both processes; they are not independent when running simultaneously.

Tunable Thermosensitive Polymer-Stabilized Liquid Crystal Smart Windows without Alignment Layers

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Keywords: Polymer-stabilized liquid crystal, Photopolymerization, Smart window.

As global warming has worsened dramatically nowadays, smart windows have become a solution to prevent indoor temperature (*T*) from rising. The development of new materials for smart windows has further enhanced their effectiveness. Polymer-stabilized liquid crystal (PSLC) is commonly suggested for thermal insulation [1] or privacy purposes in smart windows. We have developed thermally responsive PSLC smart glass with SmA–N* phase transition and *T*-sensitive properties using 1,7-bis-4-(4-cyanobiphenyl) heptane (CB7CB). The cell does not entail field stimulation, but instead self-sufficiently adjusts the transparency in response to ambient *T*, displaying grey-scale transmission variations without a polarizer [2]. The innovation is the incorporation of CB7CB with a bifunctional monomer (RM257) and a trifunctional monomer (TMPTA) in the nematic LC 8OCB to form a polymer network through ultraviolet irradiation. The resulted CLC exhibits SmA orientation along the vertically applied electric field, eliminating the need for an alignment layer. Figure 1(a) demonstrates that the inclusion of CB7CB in small quantities can significantly decrease the necessary SmA phase transition point. Figure 1(b) reveals that this device exhibits a high contrast ratio. The sample shows higher transmission in the SmA phase. As *T* increases to induce disordered orientation of LC molecules, the device becomes opaque when the LC turns into the N* phase. Figure 1(c) illustrates our proof of concept although the switching temperature around 58 °C is somewhat unpractical.

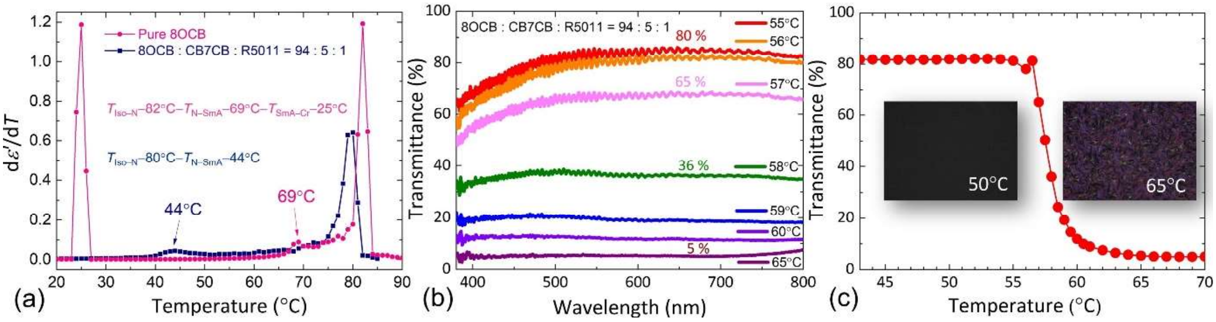

Figure 1: (a) Phase transition sequences of pure 8OCB and the uncured mixture counterpart acquired by the real-part dielectric data at 10 kHz; (b) visible transmission spectra of a 15-μm-thick PSLC at various *T*; (c) *T*-dependent average transmission of the PSLC cell obtained in the heating process. Insets: textures at $T = 50$ and 65 °C.

Acknowledgments: National Science and Technology Council, Taiwan (111-2112-M-A49-033;112-2112-M-A49-031).

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B2

Photosensitive liquid crystals

Hydrogen-bonded Multi-Mode Liquid Crystal Elastomer Actuators

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Keywords: liquid crystal elastomer, hydrogen bonding, humidity-responsive, photoactuation, shape-memory.

With the deepening exploration of biomimicry concepts, liquid crystal elastomers (LCEs) with multi-mode stimuli-responsiveness and complex shape morphing ability have become a hot topic in contemporary materials research.[1] In this context, dynamically bonded LCEs enable versatile shape programming and subsequent reversible photothermal actuation of the programmed shape, showing potential in soft robotic applications.[2] Here we present a multi-mode LCE combining shape memory programming, humidity sensitivity, and photochemical actuation properties. Our design concept is depicted in **Figure 1**. The incorporation of dynamic hydrogen bonds into the LCE imparts shape memory functionality to the photochemical actuator, allowing for arbitrary shape programming and subsequent shape morphing in the programmed state. Depending on the programmed shape, robotic applications such as light-driven grippers that can adjust their shape for grabbing different-sized objects, are demonstrated. Treatment of the film with KOH induces salt formation on the surface, rendering one side of the LCE hydrophilic and, consequently, humidity-responsive. The base-treated LCE bends in moderately humid environments, and the bending can be further controlled via the photochemical effect. The proposed multi-mode LCE exhibits complex interplay between humidity and photochemical response, combining facile control over the speed, geometry, and directionality of the movements and promising smart and adaptive bioinspired microrobots.

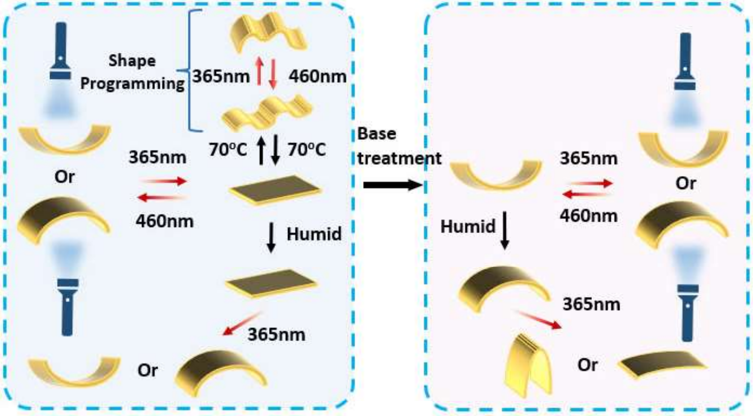

Figure 1. Schematic illustration of photochemically driven, humidity-sensitive LCE actuator with shape programming, and shape morphing property.

Acknowledgements: Research Council of Finland (Center of Excellence Programme LIBER), European Research Council (Consolidator Grant project MULTIMODAL), and Tampere University Doctoral School are gratefully acknowledged for funding and financial support.

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Ortho-fluoroazobenzenes for photoalignment

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Keywords: photoalignment, fluorinated azobenzenes, LC polymers

Azobenzene-containing liquid crystalline polymers belong to a unique class of hybrid materials combining the properties of macromolecular compounds with extraordinary optical properties of liquid crystals and photochromism of azobenzene-based materials. Polarized visible light irradiation leads to an appearance of photoinduced dichroism and birefringence in these materials. This phenomenon is called photoalignment and it can be used for the creation of materials for applications in photonics and flat optics.[1,2] In particular, the ability to create diffractive optical elements based on periodic polarization patterns are highly promising for applications in augmented reality (AR) and virtual reality (VR) technologies. Thus, understanding and manipulating photoalignment mechanisms, and understanding how they relate to the photochemical properties of the molecular building blocks used, is key to unlocking many innovative applications in different fields of optics and photonics.

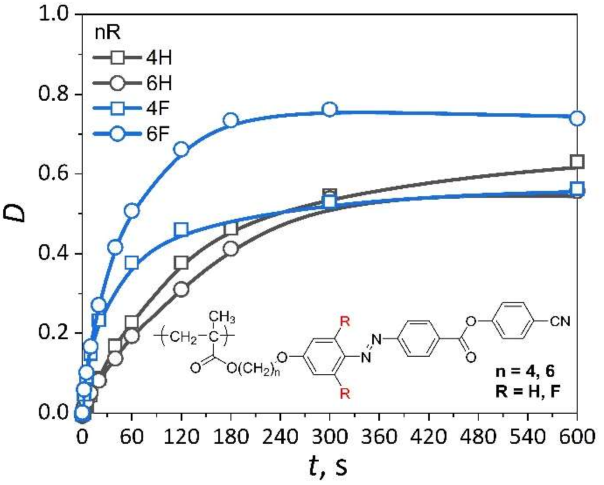

Figure 1. Kinetic curves of dichroism values and chemical structure of studied materials.

The introduction of σ-electron-withdrawing F atoms in the ortho position to the azo group leads to both effective separation of the n→π* bands of E- and Z-isomers, which opens the possibility of using these two transitions to selectively induce E/Z isomerization, and significantly increased thermal stability of the Z-isomer.[3] The effect of the unique photochemical properties of fluorinated azobenzenes has not yet been studied in the context of photoalignment processes. Thus, in this work, we explored how the lateral fluorine substituents in the azobenzene photochrome affect the process of photoalignment in comparison with the unsubstituted analogue. It has been found that *ortho*-fluorination increases the dichroism values and the speed of the photoalignment process compared with the similar azobenzene-containing polymers without lateral substituents (Fig.1). Fluorination of azobenzenes seems like a highly potent route to improve the photooptical properties of photoaddressable materials.

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Photodeformable and Multi-Functional Liquid Crystal Polymers via Ring-Opening Metathesis Polymerization

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Keywords: liquid crystal polymers, photodeformation, multifunctional, soft actuators

Photo- and multi-functional crosslinked liquid crystal polymers (CLCPs) are promising materials for designing intelligent soft actuators due to their distinct stimuli-responsive shape-changing abilities. However, chemically crosslinked LCPs are insoluble in organic solvents and infusible upon heating, which are incompatible with commonly used polymer processing methods and difficult to implement the construction of 3D actuators with alterable geometry. On the other hand, the existing mature approaches for constructing multifunctional LCPs in response to external stimuli are still hampered by the fact that some functional monomers are not accessible by direct polymerization. Therefore, the molecular design of new materials is essential for improving the processibility and functionality of LCPs.

We synthesized the linear LCPs by ring-opening metathesis polymerization (ROMP), which possessed good mechanical properties due to the high molecular weight and physical crosslinking. Linear LCPs were easily processed into 3D microchannels due to the absence of chemical crosslinking network, which presented a conceptually novel way to propel liquids by capillary force arising from photo-induced asymmetric deformation. Furthermore, the microchannels were integrated into the microfluidic chips to construct lab-on-a-chip platforms for efficient liquid transportation, mixing, fusion and separation, which effectively get rid of the external control devices and realize portable biochemical analysis.

Moreover, we propose a facile synthetic approach by combining the respective advantages of ROMP and post-polymerization modification to attain a new multifunctional LCP. ROMP is utilized to synthesize a high molecular weight reactive photo-responsive LCP precursor in the first place, which endows the precursor with good mechanical properties without further chemical crosslinking. Moreover, the existence of reactive groups renders the above LCP to undergo efficient coupling reactions with a humidity-responsive functional group via post-polymerization modification reactions, which is difficult to achieve with direct polymerization.

Acknowledgements: The authors would like to acknowledge the financial support from the National Natural Science Foundation of China (51927805, 52233001) and the Natural Science Foundation of Shanghai (20ZR1406700).

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Photophysical study of symmetric triazines substituted with 4helicenyl for application in OLED

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Keywords: OLED; Triazine; Molecules

Optoelectronic devices have brought together improvements through advances in organic semiconductors, some examples of these improved devices are organic field-effect transistors (OFETs), organic photovoltaics (OPVs) and organic light-emitting diodes (OLEDs). With this fact, one of the objectives of this work is to improve the molecular alignment between emitters for better light emission, through the classification of two triazine molecules with the same nucleus. To this end, a variety of different equipment and techniques were used.
It was demonstrated in a work that using triply phenantryl and 4helicenyl with short alkyl chains, glass transitions occurred above room temperature within the hexagonal columnar liquid crystalline state, thus resulting in a solid columnar order at room temperature [1].
Films were produced with the two molecules mentioned, through spin coating and blade coat, using chloroform as a solvent for preparing films and solutions. Comparisons also occur between molecules, such as behavioral actions, photophysical and morphological properties.

Acknowledgements: INCT/INEO, Capes, CNPq, CAPES-COFECUB (#937/20 and # Ph-C 962/20) and H2020-MSCA-RISE-2017 (OCTA, #778158).

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Photophysical study of symmetric triazines substituted with phenantryl for application in OLED

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Keywords: OLED, Triazine, Alignment

Molecules with rigid aromatic centers and flexible side chains are widely studied and tested in organic studies and tested in organic devices such as light-emitting diodes (OLEDS), field-effect transistors (OFETs) and photovoltaics. LC combines the molecular organization of crystalline systems with a certain fluidity, facilitating the process of charge and material transport. One of the goals of this work is to categorize the combination of two symmetrical triazine molecules with different side chains, so comparisons were made in relation to their behavior and their photophysical and morphological properties using different techniques, such as the production of films by spin coating and blade coating techniques, using chlorine. Spin coating and blade coating techniques, using chloroform as the solvent for film production and for analysis in solution. Observation of the photophysical processes was carried out using UV-VIS absorbance spectroscopy and photoluminescence spectroscopy. This process was repeated with the molecules separately in solution and their combination was analyzed in solution and films, by spin coating and blade coating. Heat treatments on the organization and packing properties, which was checked in a polarized light microscope (MOLP). Differential Scanning Calorimetry Scanning Calorimetry (DSC) was used to analyze the thermotropic behavior of triazine molecules individually and in combination.

Acknowledgements: INCT/INEO, Capes, CNPq, CAPES-COFECUB (#937/20 and # Ph-C 962/20) and H2020-MSCA-RISE-2017 (OCTA, #778158).

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Photophysics Analysis Assisted by Numerical Calculations: Towards OLED Efficiency

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Keywords: DFT; Photophysics, OLED efficiency

Organic molecular systems have been a hot topic of study in the scientific community due to new technological applications they can present. However, these systems hide many important non-measurable properties only accessed by numerical calculations, making use of theoretical models with various theory levels to fit a specific system. The efficiency of organic light emitting diodes (OLEDs) can be improved by the molecular ordering of the emitting molecules inside the active layer, since higher order improves charge transport, energy conversion and light outcoupling [1]. In this sense, liquid crystals can play a special role due to their self-aligning properties. Here, the photophysical analysis of perylene-based liquid crystals are assisted by numerical calculations to access the electronic distribution and localization of the frontier molecular orbitals, the influence of the magnetic field due to atomic interactions and detailed information about electronic transitions. Those analyses were performed using density-functional theory (DFT) [2], allowing the simulation of the molecular orbital surfaces and absorption/emission spectra. We were able to predict molecular systems towards more sustainable devices with higher efficiency.

Acknowledgements: INCT/INEO, Capes, CNPq, CAPES-COFECUB (#937/20 and # Ph-C 962/20), FAPESC, H2020-MSCA-RISE-2017 (OCTA, #778158).

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Photophysics of perylene derivatives in triazine host for application in OLED

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Keywords: OLED; Perylene; triazine; alignment

The latest advances with organic semiconductors have provided competitive optoelectronic devices with new functionalities, as observed for organic light emitting diodes (OLEDs), organic field effect transistors (OFETs), organic photovoltaics (OPVs) and sensors. The efficiency of these devices depends directly on the molecular ordering achieved by the active layer, since higher order improves charge transport, energy conversion and light outcoupling. In this sense, self-organizing molecules, such as liquid-crystalline materials, effectively play a role in this field. In a previous work, we demonstrated that the molecular alignment of a columnar liquid crystal (ColLC) in a diode structure improved the charge carrier mobility in five orders of magnitude and allowed electroluminescence emission [1]. Here, we investigate a triazine-based ColLC as aligning host for emissive molecules to be applied in the active layer of OLEDs, based on a work where we demonstrated the potential of the photophysical properties of liquid-crystalline triazine-based molecules for alignment-induced enhancement of light outcoupling [2]. As guest emissive molecule we investigated a thermally activated delayed fluorescent compound, which absorption band overlaps with the emission peak of the triazine-based host in order to optimize energy transfer [3]. The photophysical studies demonstrated that for 10.0 wt% concentration of the guest, the host emission is totally converted to the guest with increasing of the photoluminescence quantum yield, which is also influenced by the molecular organization of the medium. In this work we investigated the photophysical behavior of perylene derivatives in 1% wt drop casting films in a triazine (5A) host. The host's emission band coincides with good coupling with the emitters' absorption band, demonstrating good host/guest energy transfer.

Acknowledgements: INCT/INEO, Capes, CNPq, CAPES-COFECUB (#937/20 and # Ph-C 962/20) and H2020-MSCA-RISE-2017 (OCTA, #778158).

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B3

Nanostructured systems and nanocomposites

Cellulose-based nanocomposites as deterrent solutions for security applications

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Keywords: Cellulose nanocrystals, nanocomposites, anti-counterfeiting, lyotropic liquid crystals, circularly light reflection

Counterfeiting is currently the second-largest source of organized crime, disturbing all segments of society (documents, clothing, food, automotive parts, pharmaceuticals, and even electronics), reaching industry, government, and end-users. Counterfeit products have become more accurate with technology development, and deterrent anti-counterfeiting solutions are in constant demand. Structural-color-generating films from cellulose nanocrystals (CNC) nanocomposites present good properties to be used as anti-counterfeiting systems. Derived from liquid crystalline lyotropic suspensions, these photonic materials present selective left-handed circular reflection, which can be used as a covert anti-counterfeiting feature, the structural coloration that can act as an overt feature, flexibility, and response to multiple stimuli (such as relative humidity, electric field, temperature, and polar solvents) as additional covert features. [1-4] Tunning optical properties and flexibility of solid films of CNC with other cellulosic derivatives was explored by the addition of hydroxypropylcellulose (HPC) [3] and hydroxypropylmethylcellulose (HPMC) [5] in home-made and commercial cellulose nanocrystals in liquid crystalline colloidal suspension, within the biphasic regime. HPC and HPMC content allows modulating the reflected pitch value within all composite systems and induces flexibility, while HPMC gives rise to a more elaborate optical response, highly dependent on the origin of the CNC and molecular weight of the HPMC, with left-handed and “apparent” right-handed optical light reflection. These new photonic cellulose-based nanomaterials are excellent candidates as anti-counterfeiting optical variable devices.

Acknowledgments: The authors acknowledge the support of FCT-Fundação para a Ciência e a Tecnologia, I.P., in the scope of the projects LA/P/0037/2020, UIDP/50025/2020 and UIDB/50025/2020 of the Associate Laboratory Institute of Nanostructures, Nanomodelling, and Nanofabrication-i3N. European Cooperation in Science & Technology (COST) Action: CA21159 – Understanding interaction light – biological surfaces: possibility for new electronic materials and devices (PhoBioS). The authors also acknowledge PON 2014-2020 (CCI 2014IT16M2OP005), FSE, Action I.1 ”Dottorati Innovativi com caratterizzazione Industriale”, that supported financially Erica's PhD.

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Characteristics of linear and circular optical properties in different liquid crystalline phases

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Keywords: chirality synchronization, optical response, thin films, Mueller Matrix Polarimetry

In recent years chiral thin films contributed significantly to the development of multiple optoelectronic technologies. One of the most studied are organic films based on liquid crystalline phases with helical geometries, such as the B4 phase. Anisotropy of alignment in such materials causes the occurrence of unwanted linear optical effects during the examination of chiroptical response. This entanglement results in linking the optical properties of the film with its orientation, posing a major obstacle in the application of such materials.

In my work, I present comprehensive research on the liquid crystalline dark conglomerate phase (DC). Its chiral, non-linear sponge-like morphology limits the occurrence of linear effects while exhibiting extremely strong circular dichroism (CD) and circular birefringence (CB). Morphology was investigated using transmission electron microscopy (TEM) and atomic force microscopy (AFM). Optical properties were characterised by a state-of-the-art method of Mueller Matrix Polarimetry (MMP), that allowed conducting a detailed study of both linear and chiral effects in thin film with a thickness ca 10 micrometers. Obtained data confirmed the material's high chiroptical activity with a minor contribution from linear phenomena. Presented MMP results for DC phase are also compared with a MMP study of a B4 phase, conducted for a series of liquid crystalline compounds.

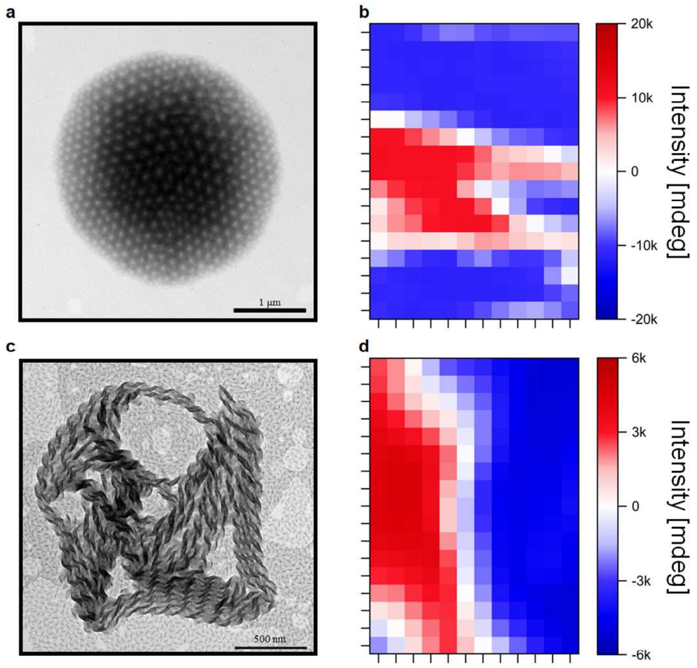

Figure 1: (a) TEM image of DC phase. (b) CD map as MMP result for DC phase. (c) TEM image of B4 phase. (d) CD map as MMP result for B4 phase.

Enhancing Circularly Polarized Luminescence: Multimodal Chirality Induction in Liquid Crystal Templated Films

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Keywords: circularly polarized luminescence, chirality, nanotubes

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Circularly polarized luminescence, an optical phenomenon where emitted light displays different degrees of left and right circular polarization, holds significant promise for optoelectronics, chiral sensing, and photonics. However, the performance of chiral emitting molecules is hindered by their inherently low excesses of one circular polarization in emitted light. Recent efforts have tackled this challenge by fabricating chiral materials in solid-state configurations, though this approach introduces difficulties in examination due to potential parasitic effects (such as birefringence, linear dichroism, circular differential scattering and selective reflection [1]). Here, we introduce a method for inducing CPL in achiral fluorescent dyes using a chiral liquid-crystalline matrix. This matrix, comprising mesogenic organic compounds, forms centimeter-sized homochiral domains during crystallization [2]. Within each domain, mesogens crystallize into chiral nanotubes with one handedness. Our approach achieves materials with luminescence dissymmetry factors reaching 0.3 (Fig. 1), a remarkable improvement over typical values for chiral organic molecules in solutions by a factor of 1000. Additionally, our results are supported by series of experiments which rule out common parasitic effects as the origin of observed chiral luminescence. These findings promise not only the development of highly efficient chiral luminescent materials but also unveil a new, universal method for CPL induction in aggregated organic dyes. This approach is complementary to existing approaches for circular dichroism induction in a chiral mesogenic matrix [2,3].

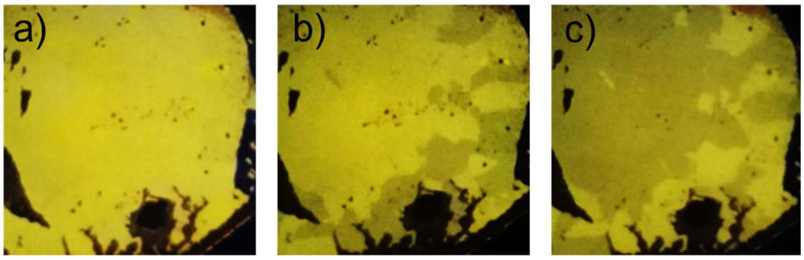

Figure 1: Circularly polarized luminescence of yellow fluorescent dye introduced into chiral nanotubes forming large homochiral domains: a) sample observed with the naked eye, b) sample observed through a left-handed circular polarizer, c) sample observed through a right-handed circular polarizer.

Acknowledgements: This research was funded in part by National Science Center, Poland under UMO-2020/39/O/ST5/03445 Preludium Bis grant.

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Growth of Nematic Domains in Quantum Dot - Liquid Crystal Nanocomposite

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Keywords: domain growth, self-assembly, nematic nucleation.

Self-assembly of nanoparticles in liquid crystals has been accomplished yielding diverse controllable structures such as foams, networks, and shells.[1] This creates a great opportunity for research and application in photonics, electronic, sensing, among others. However, before diving into the application, we need to understand the systems and their mechanism. For this, we have chosen to study the nanocomposite formed by nematic liquid crystal 5CB (4-cyano-4'-pentylbiphenyl), and quantum dots coated with diverse calamitic ligands. The initial stage of the self-assembly process is studied by high-speed video microscopy under varying cooling rates, quantum dots concentrations and coating materials. We have compared our experimental observations with simulations and noticed how the phase boundary transports the quantum dots and the nematic growth correlates with the universal growth law $L(t) \sim t^n$,[2] where L is the characteristic length of the system and n is the universal growth exponent. These results will help us to gain a better understanding of the structure formation.

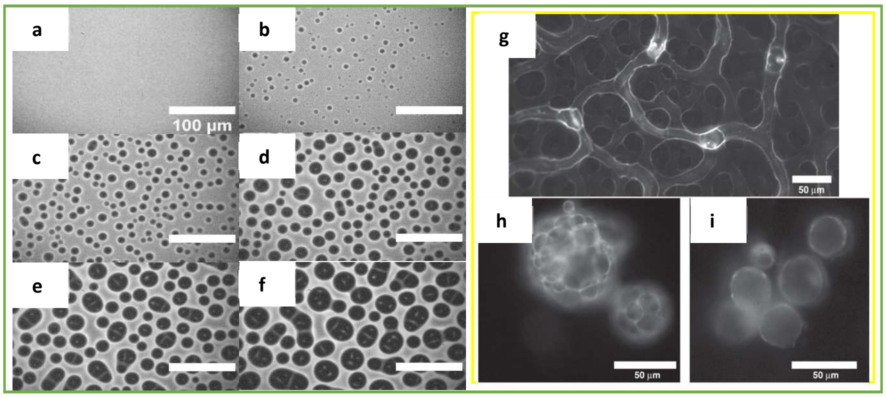

Figure 1: a-f) Nematic nucleation and growth of 5CB, g-i) Final structures: g) network, h) foam, i) shells.

Acknowledgements: We gratefully acknowledge support from the National Science Foundation (DMR-2104574).

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Lyotropic LC Phases of Isotropic Nanoparticles via Chiral Polypeptide Ligands

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Keywords: Lyotropic, nanoparticles, semiflexible polymers, synthetic polypeptides

We recently showed that anisotropic (nematic) lyotropic phases can be formed by spherical metal oxide nanoparticles (NPs) through functionalization with semiflexible polymer ligands.[1] This approach has been extended to produce chiral LC phases of the same NPs with synthetic polypeptide ligands including poly(γ-benzyl-L-glutamate) (PBLG) and poly(γ-stearyl-L-glutamate) (PSLG). At sufficiently high concentrations, ZrO_2 NPs functionalized with PBLG ligands (PBLG-ZrO_2 NPs), were observed to form lyotropic cholesteric and columnar hexagonal LC phases, while PSLG-ZrO_2 NPs were able to form both thermotropic and lyotropic LC phases, as seen by the cholesteric fingerprint textures (Fig.1). In agreement with our previous study of NPs with poly(hexyl isocyanate) (PHIC) ligands, lower critical LC concentrations were observed for the NPs when compared to the free polymer in solution. Whereas the PHIC-ZrO_2 NPs have reduced nematic order, small angle X-ray scattering (SAXS) of lyotropic solutions of the NPs with chiral polypeptides showed stronger and sharper Bragg diffraction peaks, indicating that tethering the polypeptide to the NPs results in a higher degree of positional order.

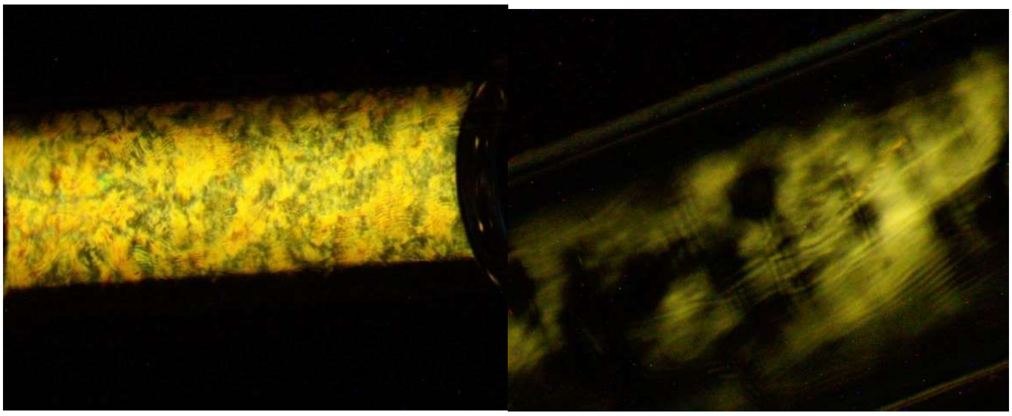

Figure 1: (left) DCM solution of PBLG-ZrO_2 NPs (right) toluene solution of PSLG-ZrO_2 NPs. oth exhibiting lyotropic cholesteric LC order.

Acknowledgements: We acknowledge the assistance of Dr. Hatem Titi with the SAXS experiments as well as support from the FRQNT Quebec Centre for Advanced Materials (QCAM/CQMF) and the Natural Sciences and Engineering Research Council of Canada (NSERC).

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Multicolored, single-piece cholesteric films

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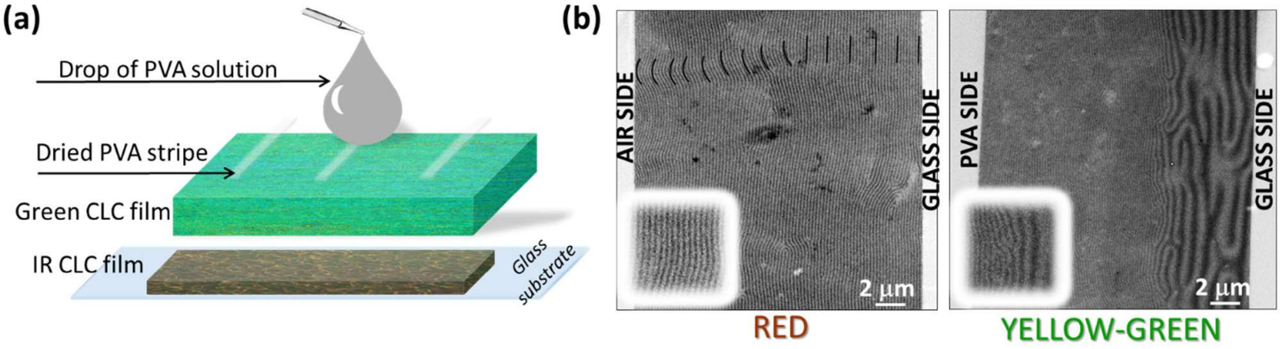
Keywords: nanostructured systems, bio-inspired LCs, optical tags, anchoring, surface tension.

Multicolored, cholesteric patterns may be observed on the bodies of insects and fish [1]. Bioinspired smart coatings might be applied to optical communication, signaling, or cryptography [2, 3]. The creation of single-piece films with continuous, hierarchical nanoscale and micrometer-scale structures, as found in nature, and accompanied by design simplicity has not been fully investigated due to the challenges inherent in such applications. The feasibility of associating various reflection colors inside a monolayer without combining discontinuous, cholesteric materials with different natural pitches is here investigated. During a diffusion-driven design process (Fig. a), we explore the distinct roles of two physical parameters: the molecular anchoring at film interfaces and the surface tension local anisotropy, which is liable to occur across the film [3, 4]. We investigate the time-dependent evolution of optical characteristics in the film plane in relation to transmission electron microscopy cross-sectional views (Fig. b). An analysis of the free, natural pitch in comparison to the material's constrained, effective pitch is discussed.



(a) The experimental cell before the design process. (b) Fingerprint textures in transmission electron microscopy cross-sections of two colored areas of the same film.

Acknowledgements: This work was financially supported by the Agence Nationale de la Recherche, France (COLEOPTIX, ANR-17-CE30-0025).

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Multiresponsive chiral nanocomposites made of plasmonic and magnetic nanoparticles in soft systems

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Keywords: liquid crystals, nanoparticles, nanocomposites, chiral systems, multiresponsive nanocomposites

The intricacy of precisely matching the organic and inorganic components, particularly in terms of chemical compatibility and nanoparticle core size, remains a major obstacle in preparation of liquid crystal nanoposites and hybrid organic-inorganic with high metal loading. [1] Although many difficulties have been surmounted, the development of systems that can be externally controlled in terms of their structural or physicochemical parameters remains a significant challenge [2].

The presentation will discuss a variety of multi-responsive system containing gold nanoparticles, iron oxide nanoparticles, and a photo-switchable diazo compound (12OAzo5AzoO12) [3],[4]. Structural and physicochemical studies will be presented showing the first supramolecular system capable of switching soft phases, created by spiropyran-modified nanoparticles, using both light and a complexing agent.

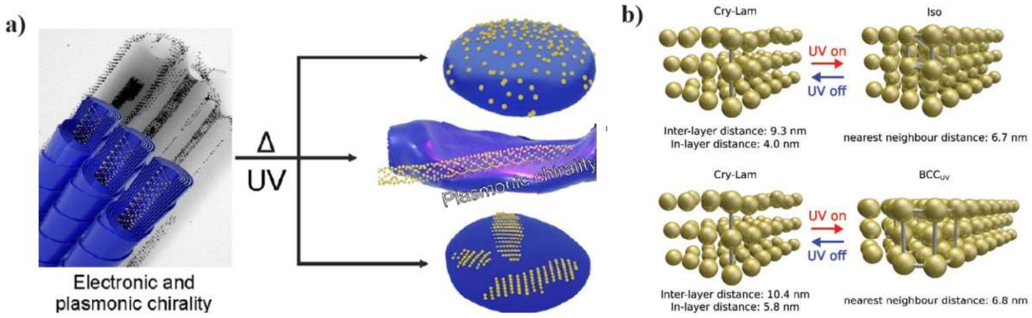

Figure 1: a) Switchable structures composed of nanoparticles and a chiral liquid crystal matrix; b) Reorganization of nanoparticles in a condensed system caused by light

Acknowledgements: The research was funded by Polish Science Center, grant number UMO-2019/35/B/ST5/04232

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Nanostructure of a Liquid Crystal due to the Presence of a Rough Buried Interface: Effect on the Transport Properties

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Keywords: liquid crystal nanowire, columnar structures, rough interface, charge transfer, conductivity

We investigate the effect that the roughness of a buried interface has on the nanostructure of a liquid crystal. This structure affects and facilitates charge transfer. The rough interface has been prepared such that the liquid crystal aligns parallel to the surface of the interface [1]. The parallel alignment includes the imperfections or openings in the rough interface that have depths that vary between 10 and 100nm [2], plus the overlap of the two materials that constitute the interface [3]. The imperfections are similar to cylindrical tubes or containers (see for example, [4]). The resulting structure is similar to a nanowire. There are many ways that the liquid crystal can go parallel inside the imperfections, but there is always a way that costs less energy to the system. We illustrate this by comparing two mechnical orientations. These evolve as a function of temperature. The way that charge transfer is achieved also evolves with temperature. A more complete picture can be determined through theoretical work. Once we obtain the orientation that gives the minimal energy, we can add the liquid crystals parallel to the interface and because they self-align, the liquid crystals that are in the next layer away from the interface will align following the molecules parallel to the interface. They will fill eventually the opening or imperfection up to its center, where there will be a disclination. When the electrons and/or the holes separate at the interface they will have a way to move through the overlap of the orbitals in this structure of parallel molecules [5] in the nanowire, and eventually reach the electrodes, increasing the efficiency. We discuss how grazing angle X-ray scattering can be used together with other characterization techniques to give us information about the alignment and the ordering of the liquid crystals.

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Novel fluctuation microscopy: spontaneous formation of the dynamic heterogeneity in swollen nematic gel near sol-gel/liquid-glass transition

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Fluctuation microscope, nematic gel, dynamic heterogeneity, visco-elastic behavior

Conventional optical microscopes visualize static inhomogeneities such as orientation, concentration, and density within a material. On the other hand, our newly developed fluctuation microscope is a new microscope that directly visualizes the distribution of dynamics within a material as "dynamic inhomogeneity" as a two-dimensional image.

UV-polymerized swollen nematic gels were prepared by mixing E44 with photo-polymerizable mesogen molecules and cross-linking agents and sealing them in a homogeneously oriented cell. We have succeeded in directly observing the "dynamic inhomogeneity" spontaneously generated during the cooling process of this swollen nematic polymer toward the glass transition temperature, as shown in Fig. 1. The image consists of 256x128 pixels, where 1 pixel = 0.8μm, and the actual size is 200μm x100μm. The pseudo-color represents the relaxation time of orientation fluctuations, which is faster for colder colors and slower for warmer colors. The spatial resolution of the developed fluctuation microscope is up to 0.4μm. The dynamic inhomogeneity images can also be recorded and analyzed as video recordings, and in this swollen nematic polymer, the dynamic inhomogeneity changes from time to time over a lifetime of a few seconds. The current video time resolution of the fluctuation microscope is about 10 ms at the fastest, and improvements are currently being made to enable even faster acquisition. On the other hand, it is also possible to perform in situ multi-frequency simultaneous dynamic Young's modulus measurements to investigate the correlation between dynamic inhomogeneity generation and macroscopic viscoelasticity. When the temperature is lowered from a sufficiently high temperature state, a remarkable divergence of the viscosity toward the glass transition temperature is observed, and a relaxation phenomenon appears in the dynamic viscoelasticity. Furthermore, it was also found that the behavior of this relaxation phenomenon changes significantly when the density of the gel mesh is increased by adding a cross-linking agent. It is obvious that there is a strong correlation between this viscoelastic relaxation phenomenon and the generation of dynamic inhomogeneity mentioned above, and we are currently conducting quantitative analysis and clarifying the mechanism.

Thus, the "fluctuation microscope" can visualizes the spatial image of "dynamic heterogeneity" in various materials, especially in soft matter and biomaterials, regardless of the degree of symmetry or randomness. Therefore, it is expected to be a useful principle and technique for characterization of food, pharmaceuticals, medical testing, and clinical applications in the future.

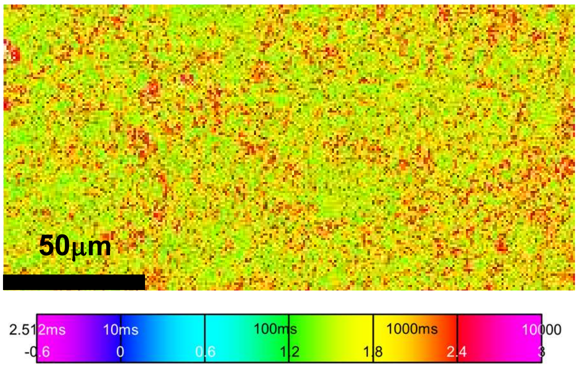

Fig.1 2D Image of dynamic heterogeneity.

Out-of-equilibrium transport in liquid crystal: new routes to particle assembly

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Keywords: nematic, nanocomposite, domains, self-assembly, non-equilibrium transport

Nanoparticle dispersal in a liquid crystal host phase can yield surprising results. The simple addition of anisotropy to a host solvent means that particles can experience a steric solubility effect - potentially transporting them in interesting ways. Recently our group has investigated what happens when an isotropic phase containing dispersed nanoparticles passes through the nematic phase transition. The resulting non-equilibrium transport of particles can be exploited to create a remarkable variety of structures including shells, foams, and gels [1] with the addition of suitable ligands [2].

In this talk I will present results from this project, in particular focusing on new work in which we examine the fundamentals behind this transport process. I will describe experiments focused on nematic domain growth and a new model by the Atherton group that describes particle transport at a moving phase boundary. This model and supporting experimental data reveal different parameter regimes where soliton-like pulses of particles surf the phase boundary or where the interface sweeps particles from one domain to another [3].

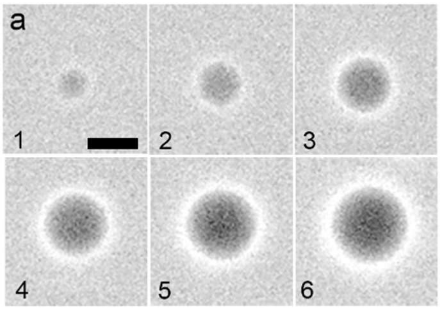

Figure 1 – Quantum dot transport at a moving nematic domain boundary (bar = 10 μm)

Our work may have broad impact. Out-of-equilibrium processes drive many of the transport mechanisms that lead to biological structure: active transport in the cell via energy-consuming molecular motors, morphogenesis in the developing embryo, or molecular and cellular organization through chemotaxis. Non-equilibrium transport is emerging as a new paradigm for materials design, where transport in chemical gradients or at phase boundaries provides unexpected routes to assembly.

Acknowledgements: This material is based upon work supported by the National Science Foundation under Grant No. DMR- 2104575.

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Performance and architecture of acrylate-based liquid crystal elastomers doped with 2,1, and free azo dyes

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Keywords: photomechanical, thermomechanical, LCE, stress, network, architecture

Azo acrylate liquid crystal elastomers are promising photomechanical materials, capable of doing mechanical work when illuminated. Azo dyes incorporated into the network undergo photoisomerization, resulting in macroscopic shape changes of samples. In typical samples, the azo moiety is covalently bonded at both ends into the network. Mechanisms contributing to the bulk shape change are a disruption of nematic order by the formation of the more compact *-cis* isomers, and a directional stress due to shortening of the aligned azo dye molecule due to the *trans-cis* isomerization. To assess the relative contributions of these mechanisms, we have prepared samples where the azo moiety is covalently bonded at both ends (2 azo), at one end (1 azo), and~~.~~ not attached to the network (free azo).

In this talk, we report the results of measurements of photo- and thermo-mechanical stress on these three types of samples and compare their performance.

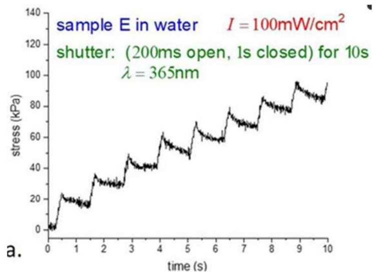

Figure 1: Photostress vs. time

Acknowledgements: US Office of Naval Research through the MURI on Photomechanical Material Systems (ONR N00014-18-1-2624).

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B4

Supramolecules

Nanoarchitectonics of Heterocoronene based Discotic Liquid Crystal Monolayer.

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Keywords: Self-assembly, free-standing monolayer, aggregation, Nanoarchitectonics

Understanding and controlling the molecular alignment of discotic liquid crystals (DLCs) is essential for their application in devices. This study investigates how surface pressure shapes molecular nanoarchitectures in oxadiazole-modified heterocoronene based discotic liquid crystal monolayer at the air-water interface[1]. Surface manometry and Brewster angle microscopy reveal the dynamic evolution of these structures. UV-visible and photoluminescence spectroscopies confirm the J-type aggregation of molecules in the solution[2]. The DLC molecules form a stable monolayer at the air-water interface. The monolayer collapses at a surface pressure of 30 mN/m. Interestingly, the heterocoronene based DLC molecules form a stable free-standing monolayer film held only by non-covalent supramolecular interaction[3]. The free-standing films can be lifted directly from the water surface onto circular rings and TEM grids, expanding their potential applications and versatility in device fabrication and manipulation. These results provide a facile method for preparing DLC films and their applications in nanoscale electronic devices.

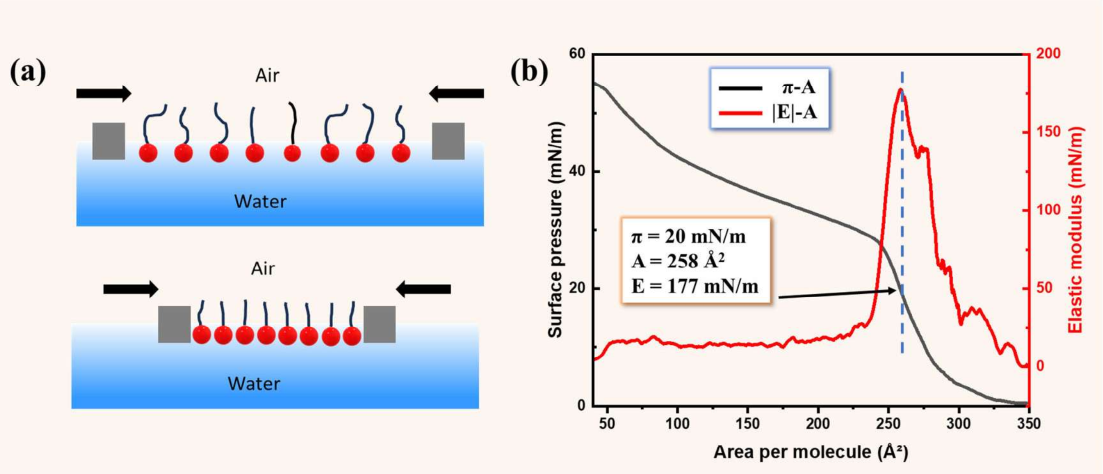

Figure 1: (a) Formation of monolayer by Langmuir-Blodgett method at air-water interface upon barrier compression, and (b) Surface pressure vs area per molecule isotherm and its corresponding elastic modulus.

Acknowledgements: A.N. thanks the Science and Engineering Research Board (SERB), Govt. of India (GoI), and the Department of Science and Technology (DST), GoI, for the research grant. H.P. acknowledges the Ministry of Education through Prime Minister's Research Fellows (PMRF) funding (PMRF-ID: 2702856) for his research fellowship.

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Temperature-dependent hole mobility in supramolecular systems

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Keywords: Discotic liquid crystal, hole mobility, charge transport, self-assembly

A supramolecular system is a self-assembling system of molecules or molecular subunits that form through intermolecular interactions. The charge transport in such a self-organizing supramolecular system is of utmost importance as they render their potential for optoelectronic and organic electronic applications. Herein, the temperature-dependent hole mobility in phenazine-fused-triphenylene and pyrene-thiophene-based discotic liquid crystals has been investigated using the time-of-flight (ToF) technique. Both the supramolecular systems exhibited hole mobility in the order of 10^{-4} $cm^2V^{-1}s^{-1}$. The hole mobility increases with increasing temperature following an inverse power law: $\mu_h(T) = \mu_0 T^n$, where n is the exponent. Owing the increasing hole mobility, such materials can overcome the limiting factor of open circuit voltage for optoelectronic devices against their poor efficiency at higher temperatures. Within the scope of this study, the underlying mechanism of charge transport is explained in such supramolecular systems.

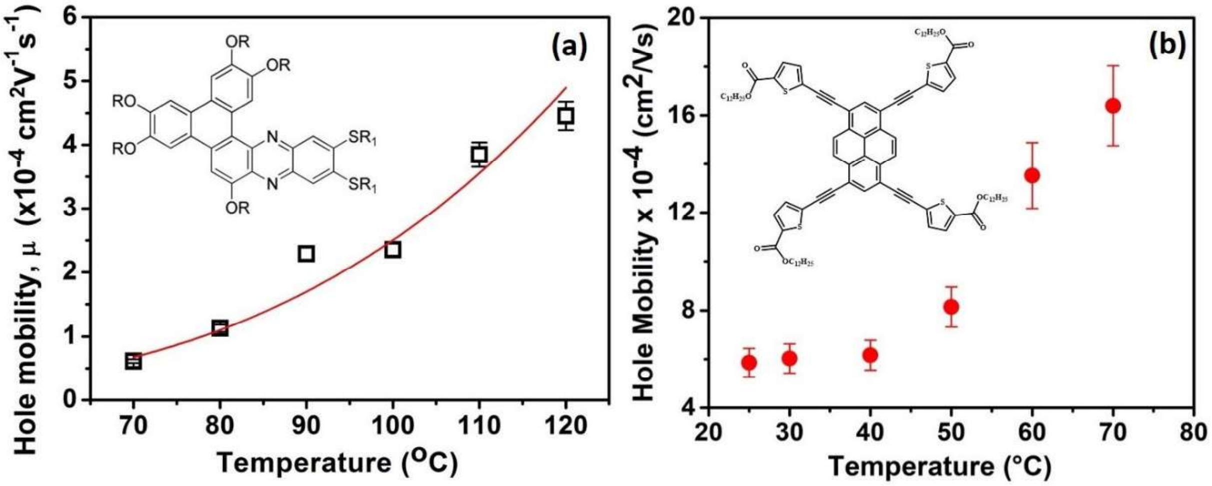

Figure 1: Temperature dependent hole mobility of (a) phenazine-fused triphenylene and (b) pyrene-thiophene-based discotics.

Acknowledgements: D.P. Singh is thankful to ULCO for financial assistance. S. K. Pal thanks DST-SERB (CRG/2019/000901/OC) for the funding assistance.

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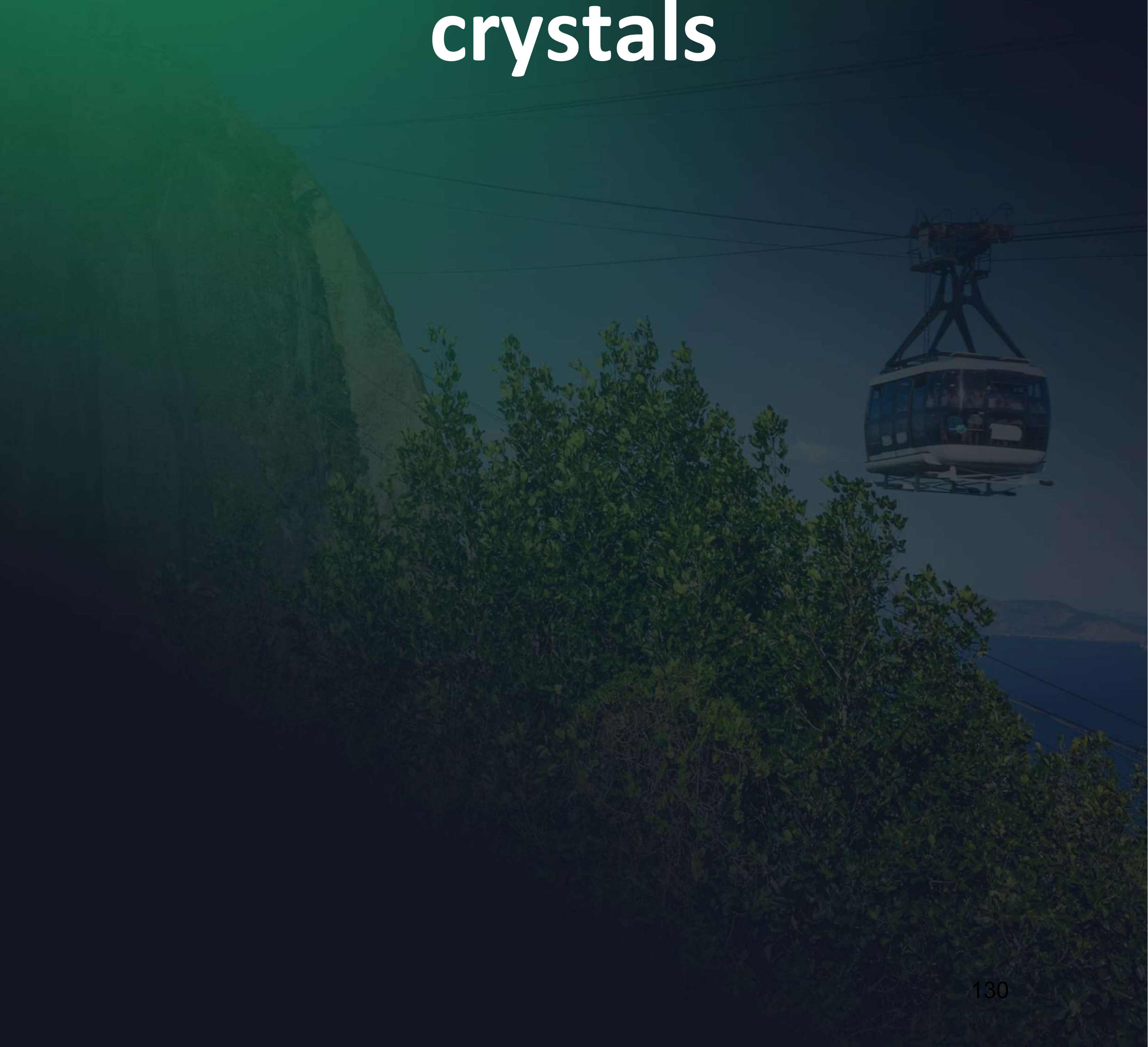
B5

Biological and bio-inspired liquid crystals



Complex Smectic Phases in Polymer Grafted Shape-Uniform Cellulose Nano-Crystals

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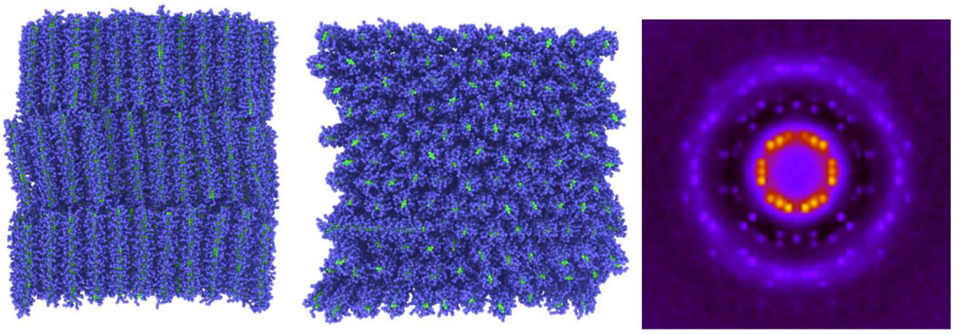
Keywords: (Polymers, LCs, Self Assembly, Complex Smectics, Cellulose)



The effect of short chain grafting on the liquid crystalline (LC) ordering of nano-crystals is investigated using molecular dynamics simulations of a coarse-grained grafted nano-rod model. Monodisperse nano-rods, with aspect ratios typical of cellulose nano-crystals (CNCs) are grafted randomly with oligomers at different grafting densities. LC ordering depends non-trivially on grafting density as the effective nano-rod shape and softness is modified. Ungrafted rods exhibit Nematic and tilted Smectic-C phases. At 25% grafting, the addition of a few side chains entirely supresses Smectic order and instead a persistent Nematic phase is favoured. Intermediary grafting, around 50%, results in a Nematic and the reappearance of tilted Smectic-F phases. Heavier grafting facilitates direct transitions to either Smectic-I with extreme tilt (75%) or an un-tilted Smectic-B (100%). Such behaviour falls outside of current hard or soft-rod descriptions of phase-transitions in rod-like LC systems and points to undiscovered LC behaviour in both shape-purified grafted/un-grafted CNCs.

Acknowledgements: The authors wish to thank the EIC Pathfinder Open Grant INTEGRATE (https://www.integrate-pathfinder.com) and Dr Patrick Davison and Dr Hendrik Meyer for helpful discussions.

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Intercellular friction and motility drive orientational order in cell monolayers

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Keywords: intercellular friction, solid-liquid transitions, nematic and hexatic order, topological defects, cellular extrusion

Cells collectively migrate and form spatiotemporal patterns in many biological processes, including embryonic development, wound healing, and cancer metastasis. In this work [1], we use a multiphase field model of deformable, motile cells to numerically study the role of intercellular friction in tissue dynamics. Such friction endows the tissue as a whole with a finite viscosity, which enhances velocity correlations. We find that varying friction and motility drives a solid-liquid transition. Furthermore, near the transition boundary, we observe the emergence of nematic order of cell deformations driven by aligning cellular flows. We also show that hexatic and nematic order are tightly coupled and propose a mechanical-geometric model for the colocalization of +1/2 nematic defects and 5-7 disclination pairs -- the structural defects in the hexatic phase. Furthermore, +1/2 nematic defects coincide with regions of high cell-cell overlap, suggesting that they may mediate cellular extrusion, which has been found experimentally [2]. Our results delineate a mechanical basis for the recent observation of nematic and hexatic order in multicellular collectives in experiments and simulations [3] and pinpoint a generic pathway to couple topological and physical effects in these systems.

Acknowledgements: A.H. and M.C.M. were supported by the NSF Grant No. DMR-2041459. This research has received funding (B. L.) from the European Research Council under the European Union's Horizon 2020 research and innovation program (Grant Agreement No. 851196).

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Lyotropics: the bilayer polar / apolar interface

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Keywords: lyotropic symmetries, phase transitions, biomembranes, pores in membranes

My work with lyotropic systems (surfactant / water / additives) started in 1976 at the new X-ray Crystalography lab of the Institute of Physics, in collaboration with the Institute of Chemistry, both of USP. For several decades our work aimed to grasp physico-chemical properties on both self-aggregation and curvature of the polar / apolar interfaces, using the simple concept of geometrical surfactant parameter, and investigating phase transitions as a function of concentrations and temperature. Main work was done with molecules with a single hydrocarbon chain, as previously reviewed [1, 2]. On the other hand, my work on lyotropics of biological interest started in 1992, in collaboration with biophysical groups, and our work on biomimetic membranes resulted in a recent review paper [3]. In this invited paper for ILCC 2024 I advance in another direction, to get information from the use of molecular dynamic (MD), possible to be made for bilayer structures. The two types of basic lyotropic symmetries (cylindrical / lamellar) have their director orientation parallel and perpendicular to a magnetic field easily defined by NMR, and the transition between them, either by chemical changes or temperature variation, constitutes a still unsolved problem [1, 2]. It has been observed that the quadrupole splitting of deuterium in nematic discotic anionic lyotropic liquid crystals is several times bigger than the value observed in cationic mesophases. Measurements of quadrupole splittings and longitudinal relaxation times, together with MD calculations of bilayers indicate [4] that the observed difference can be mainly attributed to a preferential orientation of deuterium in molecular groups at the anionic interface. A more recent MD study [5] was made on the lamellar phase of lyotropic liquid crystals differing in the degree of hydrophobicity, and data obtained by MD simulations show good agreement with the results of real experiments. Finally, a focus on MD results of hydrophilic pores in membranes [6] allowed crossing the bridge from lyotropic liquid crystals to Biomembranes without proteins. The detailed analysis of the abnormal melting transition in biomimetic membranes with pores previously made [3] can be now compared with parameters of the MD simulations, to explain the anomalous melting behavior of the anionic phospholipid DMPG (dimyristoyl phosphatidyl glycerol) and its permeability.

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Xanthan-based photonic materials: from thickening agent to structural color

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Keywords: Lyotropic liquid crystals, cholesteric phase, polysaccharides, selective reflection

In recent years, photonic films made from cellulose nanocrystal suspensions have drawn considerable research interest due to their potential applications in sensing, coloring, and actuation, as well as their low weight and high sustainability.[1] The origin of their photonic properties is the periodic modulation of the optical axis and thus the effective refractive index, which is due to the cholesteric structure trapped during the drying process of the lyotropic liquid crystal. Thus, high-quality films need to be well-aligned and exhibit a defect-free structure – properties which are still challenging to achieve.

Our work reveals now that another natural polysaccharide, i.e. xanthan which is typically used as thickening agent, is even better suited for the fabrication of photonic films. Maret et al.[2] were the first to show that enzymatically hydrolyzed xanthan forms a lyotropic cholesteric phase. Later on, Livolant[3] reported that the cholesteric phase of the xanthan/water system selectively reflects circular polarized light. We will now demonstrate that by applying the right treatment, the lyotropic cholesteric phase of xanthan can readily be transformed into colorful dried films which selectively reflect left-circular polarized light. We will correlate the treatment conditions, the properties of the cholesteric phase, the gelation and the dried films to elucidate why structural integrity is easier achieved and tuned in dried xanthan films compared to dried cellulose nanocrystal films. Furthermore, we will discuss an interesting "self-doping" effect which occurs in the treated xanthan/water system.

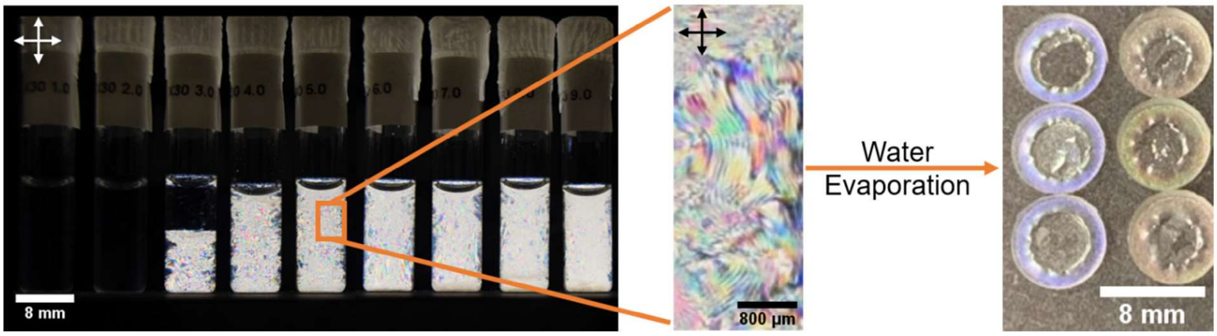

Figure 1: From left to right: Aqueous mixtures with 1 to 9 wt% of treated xanthan between crossed polarizers. Fingerprint texture of a sample with 5 wt% of treated xanthan between crossed polarizers. Dried xanthan films exhibiting selective reflection.

Acknowledgements: This project is supported by the Ministry of Science, Research and the Arts Baden-Württemberg. We thank Volkmar Vill and Jan Lagerwall for fruitful discussions.

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B6

Phase, structure and ordering

All-atom simulations of CB6OIBeOn: a progress report

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Keywords: Molecular Dynamics simulation, phase behaviour

Abberley et al.[1] have reported fascinating phase behaviour for 4-[{[4-({6-[4-(4-cyanophenyl) phenyl]hexyl}oxy)phenyl] methylidene}amino]phenyl-4-alkoxy-benzoates (CB6OIBeOn), where n is the carbon number of the terminal alkyl chain. The molecular structure for n = 6 is shown in Figure 1. For $n \leq 6$, cooling yielded the phase sequence I→N→NTB→HexI→K (crystal) whereas for $n > 6$, the sequence was I→N→SmA→SmAB→ SmCTB→HexI→K. The spontaneous formation of helical structures can render the phases as chirality.[1,2]

With the hope of casting lighter on the molecular organisation in these phases and the driving forces for their formation, we have embarked on a Molecular Dynamics simulation study. We have simulated 700 molecules, using the the General AMBER Force Field (GAFF)[3], at a pressure of 1 bar.

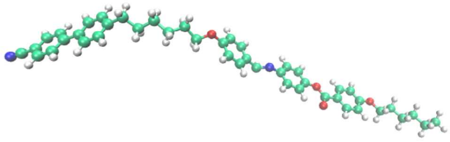

Figure 1: Molecule structure of $CB6OIBeO_6$

To date we have observed the nematic phase N and the twist-bend nematic phase N_{TB} for $n = 6$, as shown in Figure 2. We are hopeful that on further cooling we shall observe the HexI phase and that studies on molecules for $n > 6$ will allow us to analyse the exotic smectic phases reported.

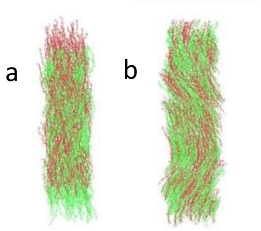

Figure 2: Simulation snapshots of 700 $CB6OIBeO_6$: (a) shows a nematic phase at 520K and (b) shows a twist-bend nematic phase at 420K with different angle colouring between the long axis of molecules and y axis. The colouring reflects the ordering of the long axis of the molecules along the director.

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Liquid crystal-based low-cost optical cell for the detection of complex biomolecules

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Keywords: Liquid crystal, interfacial interactions, polarized micrograph, proton detection, hydrolysis.

Typically, the detection methods of chemical species in sensing platform involves the use of labelling agents. Even though it is selective, the process is complex and time consuming. Liquid crystals (LC) are sensitive and rapidly responsive to the presence of any foreign species. When a LC layer interacts with aqueous (ionic surfactant) solution, there is homeotropic alignment of the director orientation due to the anisotropic interactions at the interface. This leads to the dark birefringence patterns observed in polarised microscope under cross polarisation[1]. In the presence of H^+ in the aqueous layer, the LC orientation is distorted resulting in a change of the birefringence patterns in the polarised micrographs[2, 3]. We have prepared an optical cell where the aqueous solution can interact with the LC layer confined within micrometre sized grids. The flow arrangement and the associated mass transfer process is optimised for enhanced interaction. The elastic interactions of the LC layer with H^+ released from the enzymatic hydrolysis of the Penicillin at the interface distorts the director orientation, and the birefringence pattern is captured with polarised microscope (cross-polarisation) as shown in the figure 1. There is a correlation between the polarised micrographs and the concentration of the H^+, which forms the basis of detection principle. The present method can be used for recognition of (bio-) chemical reactions releasing H^+. The developed optical flow cell is inexpensive, less than $1. The outcome of the present work may be useful for technological adaption and prospective use in point-of-care devices and field test kits.

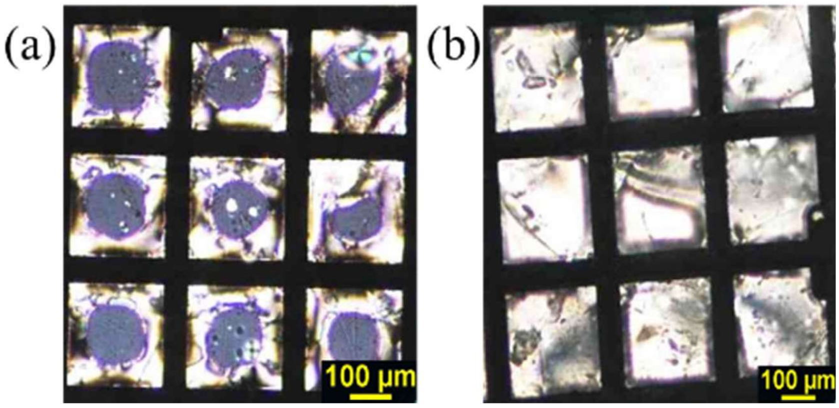

Figure 1: Polarized micrographs of the liquid crystal in the developed optical cell when 1mM Penicillin G solution is passed on the 100 mesh grid which is (a) not immobilized with Penicillinase (b)immobilized with Penicillinase.

Acknowledgement: This work was supported by a grant from the science and engineering research board (SERB), Department of science and technology, Government of India, Sanction order: CRG/2021/001218, dated December 30, 2021.

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Mix And Match: Twist-Bend Nematic Behavior In Liquid Crystal Dimer Mixtures

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Keywords: twist-bend nematics, LC mixtures, LC dimers, phase diagram, Differential Scanning Calorimetry (DSC), Polarized Optical Microscopy (POM)

The nano-scaled helical structure of the twist-bend nematic (N_{TB}) phase offers promising applications in advanced polarization technologies, light modulators, and other devices based on ultra-fast electro-optical switching (*1*). Current research suggests that molecular curvature is essential for the formation of the N_{TB} phase (*2*), prompting efforts to synthesize new liquid crystal dimers to improve their properties. This enhancement focuses on maintaining the molecular bend, which is linked to helical spacing and is directly proportional to switching time. However, some of these efforts, such as introducing thioether linkages, have inadvertently led to diminished technological parameters, such as a short and high temperature range for the N_{TB} phase and a dependency on phase transition dynamics in forming the N_{TB} phase.

In this study, we address the challenge of achieving optimal technological parameters by combining N_{TB}-forming dimers derived from the archetypal CB7CB into binary mixtures. Our approach is twofold:

- We utilize two liquid crystalline materials, one exhibiting the twist-bend phase and the other not, or only during supercooling. In such cases, determining the phase transition temperature using optical microscopy or differential scanning calorimetry becomes challenging.
- The second strategy involves mixing two materials that both exhibit the N_{TB} phase to improve the mixture's technological parameters. This includes expanding the temperature range of phase occurrence, lowering phase transition temperatures, and reducing the helix pitch in the material, consequently shortening the system's switching time.

The materials investigated are characterized by similar mesogenic groups but differ in the functional groups within the bridges connecting the central alkyl chain to the mesogens. Differential Scanning Calorimetry (DSC) and Polarized Optical Microscopy (POM) were used for the preliminary investigation.

Acknowledgements: K.M. and B.L. thank the National Science Center for funding through project no. 2020/39/O/ST5/03460. This work has been made possible through the financial support of the Polish National Agency for Academic Exchange through project no. BPN/PRE/2022/1/00053/U/00001.

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Size-Disperse Colloidal Liquid Crystals: Fractionation, Demixing and High-Pressure Self-Assembly

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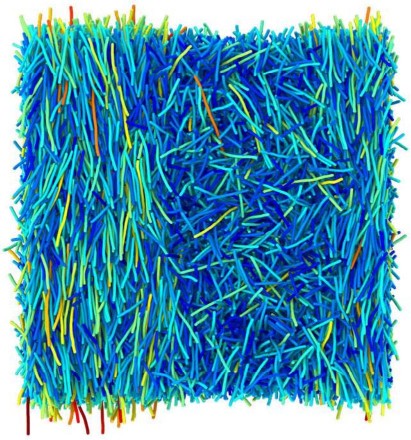
Keywords: (Polydispersity, Self-Assembly, Cellulose, MD Simulations)



Polydispersity is ubiquitous in lyotropic LCs composed of nanorods or stiff polymers but its subtle impact on the LC phase behavior and material performance is poorly understood and often overlooked in both experiment and theory. Control of a suspensions' polydispersity through the molecular weight distribution is of key importance to promote crystallization, to improve the electronic conductivity of percolated rod networks or to optimize the rheo-mechanical response of complex fluids. Inspired by recent observations of multiphase splits in cellulose nanocrystal (CNC) suspensions we combine Onsager theory [1] with large-scale Molecular Dynamics computer simulation to study LC order of length-disperse colloidal rods. We find evidence of a demixing of a polydisperse nematic fluid driven by subtle size partitioning among the two daughter phases and facilitated by the weak backbone flexibility of the colloids. In practice, this means that an isotropic-nematic-nematic triphasic split may occur over a relatively narrow bandwidth of parental polydispersities around 20-25 %. This range coincides with typical values reported for a large class of size-disperse CNC suspensions [2]. Finally, we discuss the fate of strong size disperse liquid crystals at high pressure where a competition between smectic and columnar order is expected.

Acknowledgements: The authors are grateful to Wim Thielemans (KU Leuven, Belgium) for inspiring discussions on size dispersity effects in CNC suspensions.

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Tunable templating of photonic microparticles via liquid crystal order-guided adsorption of amphiphilic polymers in emulsions

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Keywords: double emulsions, cholesteric liquid crystal, photonic microparticles**,** focal conic domain, amphiphilic

Multiple emulsions typically rely on amphiphilic molecules to maintain stability, integrating the chemical properties of the different phases in contact. While conventional wisdom assumes that the orientational order of liquid crystal (LC) phases does not affect the stabilizer, our research demonstrates for the case of amphiphilic polymer stabilizers, that this impact can be considerable [1-2]. The mode of interaction between stabilizer and LC changes if the latter is heated close to its isotropic state, initiating a feedback loop that reverberates on the LC in form of a complete structural rearrangement. Exploiting this phenomenon, we dynamically adjust the configuration of cholesteric LC shells, transitioning from a radial helix with spherically symmetric Bragg diffraction to a focal conic domain configuration with intricate optics. Furthermore, we template photonic microparticles from the LC shells by photopolymerizing them into solids, retaining any selected LC-derived structure. Our findings shed new light on LC emulsions, prompting a reassessment of stabilizer behavior when in contact with long-range ordered phases, and offering exciting possibilities for photonic elements with broad applications.

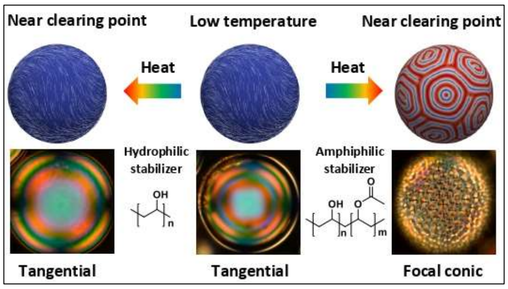

Figure 1: Numerical Simulation results (first row) and transmission POM images of cholesteric liquid crystal shells undergoing different alignment transitions with hydrophilic stabilizer or amphiphilic stabilizer when they were heated to close to the isotropic state.

Acknowledgements: This research was funded by the Luxembourg National Research Fund (FNR), the Leverhulme Trust and International Academic Fellowship and the University of Strathclyde, Sir David Anderson Bequest Award (Y.H.). We thank J. Baller for the access to the DSC. We thank Yiwei Wang for sharing his numerical code for nematic shells from ref.1.

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Unravelling the Molecular Dynamics and Intermolecular Interactions in Nematic Twist-Bend Phase: Experimental and Computational Insights

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Keywords: twist-bend nematics, LC dimers, dielectric spectroscopy, Infrared & Raman spectroscopy, DFT calculations

The nematic twist-bend phase in liquid crystal dimers presents a fascinating interplay between molecular dynamics and short-range intermolecular interactions. Through a comprehensive investigation combining experimental techniques including dielectric, infrared, and Raman spectroscopy alongside Density Functional Theory (DFT) simulations, we delve into the formation and stabilization mechanisms of this intriguing phase. Our study focuses on different liquid crystal dimers featuring cyanobiphenyl, difluoroterphenyl and naphthalene mesogenic groups.

Dielectric spectroscopy spanning frequencies from 10 Hz to 1 GHz unveils the molecular orientational dynamics in both nematic and twist-bend phases. We discern two distinct relaxation processes corresponding to the precessional rotation of molecular dipoles and the end-over-end rotation, shedding light on their behavior across phase transitions. These findings are corroborated by IR spectroscopy, which elucidates longitudinal correlation of molecular dipoles, and further supported by DFT simulations. In parallel, polarized beam infrared spectroscopy unveils changes in molecular orientation and intermolecular interactions, particularly accentuated in the nematic twist-bend phase. The transition from the nematic to twist-bend phase reveals a notable decrease in absorbance for longitudinal dipoles, attributed to anti-parallel axial interactions, followed by an increase in absorbance for transverse dipoles. DFT calculations unravel the influence of intermolecular interactions, showcasing the role of hydrogen bonding and π-π orbital interactions in stabilizing the twist-bend phase.

Moreover, simulations and experimental data converge on the significant increase in intermolecular interactions as the system transitions from the nematic to the twist-bend phase. The formation of heliconical bond order correlates strongly with the twist-bend molecular conformation, driven by short-range positional order and longer-range bond order. Our study underscores the importance of molecular geometry and intermolecular interactions in elucidating the intricate dynamics of the nematic twist-bend phase, paving the way for further advancements in liquid crystal materials design and applications.

Acknowledgements: K.M. and B.L. thank the National Science Center for funding through project no. 2020/39/O/ST5/03460.

C

Ferroelectric materials

C1

Symmetry, chirality, polarity

Novel Longitudinal Ferroelectric Polar Smectic Phases

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Keywords: Novel polar smectic phase. Spontaneous symmetry breaking.

In 2017, the ferroelectric counterpart (N_F) to the classic paraelectric nematic phase (N) was discovered [1, 2], and since then the N_F phase has become the hottest area in liquid crystal science currently. In the process of studying the N_F phase in rod-like molecular systems, polar variants of the traditional smectic A (SmA) phase with the polarization vector parallel to the layer normal were discovered [3, 4] suggesting that polar variants of the traditionally apolar LC phases are experimentally possible.

In this talk it will be demonstrated that various longitudinally polar equivalents of both the paraelectric SmA and SmC phases are indeed formable. These phases show exciting properties such as ferroelectricity and anti-ferroelectricity as well as spontaneous chiral symmetry breaking resulting in a fluidic LC phase that selectively reflects visible light. We will also shed light onto the coupling of polar and LC transitions in LC materials through emergent phase behavior via mixture formulation whilst also demonstrating mixtures exhibiting room temperature N_F phases.

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C2

Ferroelectric nematic materials

A Computational Study on the Mechanism of Ferroelectric Nematic Liquid Crystals

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Keywords: ferroelectric nematic liquid crystals, molecular simulation, machine learning

In the past few years, there have been a number of reports on nematic liquid crystals (LCs) with large dielectric constants above 10,000 that exhibit ferroelectricity; these are called ferroelectric nematic (NF) LCs.[1],[2] The NF phase has attracted much attention from many LC researchers due to its unique physical properties.[3],[4],[5] While several important physical properties of NF LCs have been well understood and some original applications based on NF LCs have been developed, the mechanism and origin still remain to be elucidated.

For further understanding of NF LCs, molecular simulation can be helpful tool to provide additional insights at the molecular level. Our recent molecular simulation studies[6] yielded important results that reveal the mechanism of NF LCs. The relationship between the orientational structure and dynamics will be discussed in the presentation.

Also, the informatics approach based on machine learning is one of the important tools to design new molecule that exhibits the NF phase. We developed a machine learning model to predict whether a molecule can exhibit the NF phase and proposed the essential feature of NF LCs, and they will be introduced.

Acknowledgements:

This work was partly supported by the JST-CREST Program (JPMJCR23O1).
The computations were partially performed at the Research Center for Computational Science, Okazaki, Japan (Project: 23-IMS-C038).

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Active state and optical manipulation of polar nematic droplets

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Keywords: ferroelectric nematic, active system, interfacial instabilities

Active matter systems, such as bacterial colonies in biology, or active membranes, are composed of constituent components that consume energy and drive the system to exhibit complex behavior [1].

We present studies of a new state of two-dimensional artificial active matter, where the constituent components are droplets of ferroelectric nematics. In the liquid bridge geometry, we observed that an electric field-induced surface instability results in the fragmentation of droplets [2]. This process gives rise to the creation of distinct "particles". Moreover, these particles show a high degree of mobility at a specific frequency and voltage range. We reveal the relationship between the emerging motion and the shape of the particles, and we make a comparison to other active matter systems.

Furthermore, we present an optical method, that allows us to manipulate the shape and the position of the polar nematic droplets.

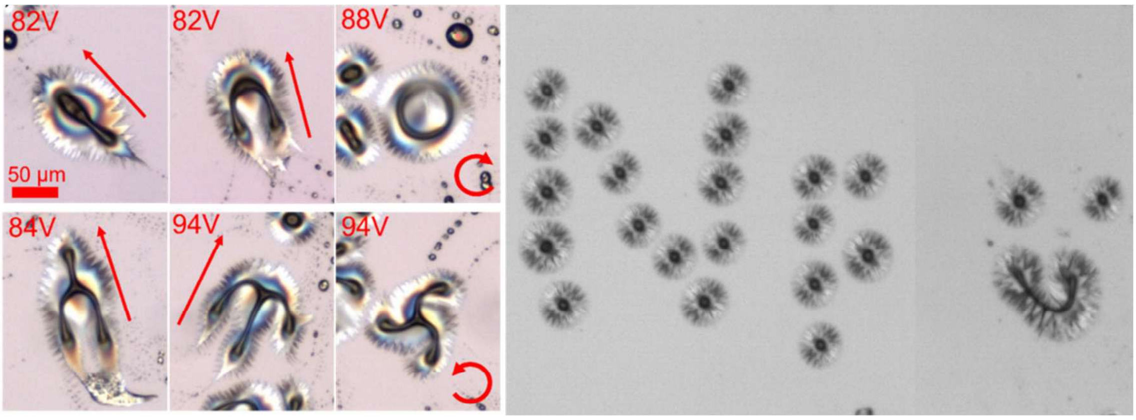

Figure 1. (left) Snapshots of the moving ferroelectric nematic droplets in the active state. (right) Ferroelectric nematic droplets arranged in a structure.

Acknowledgements: This work was supported by NSF DMR 2210083, by NKFIH FK142643, EIG CONCERT-Japan project 'FerroFluid' (2023-1.2.1-ERA_NET-2023-00008) and by ÚNKP-23-3 New National Excellence Program of the Ministry for Culture and Innovation from the source of the National Research, Development and Innovation Fund.

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[2] M.T. Máthé, et al., Sci Rep **13**, 6981 (2023)

A step toward systematization of polar nematic phases

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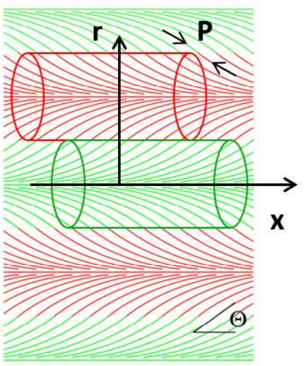
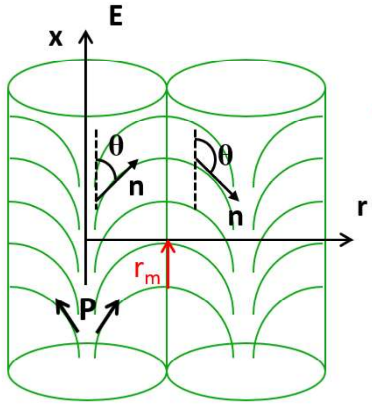
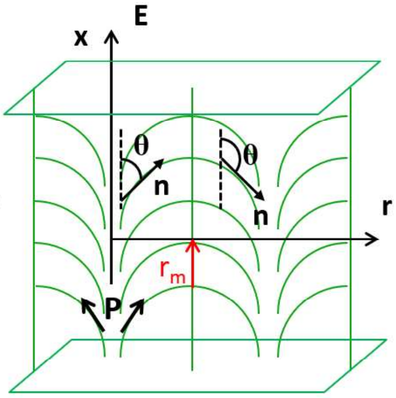
Keywords: ferroelectric and antiferroelectric nematics, splay phases



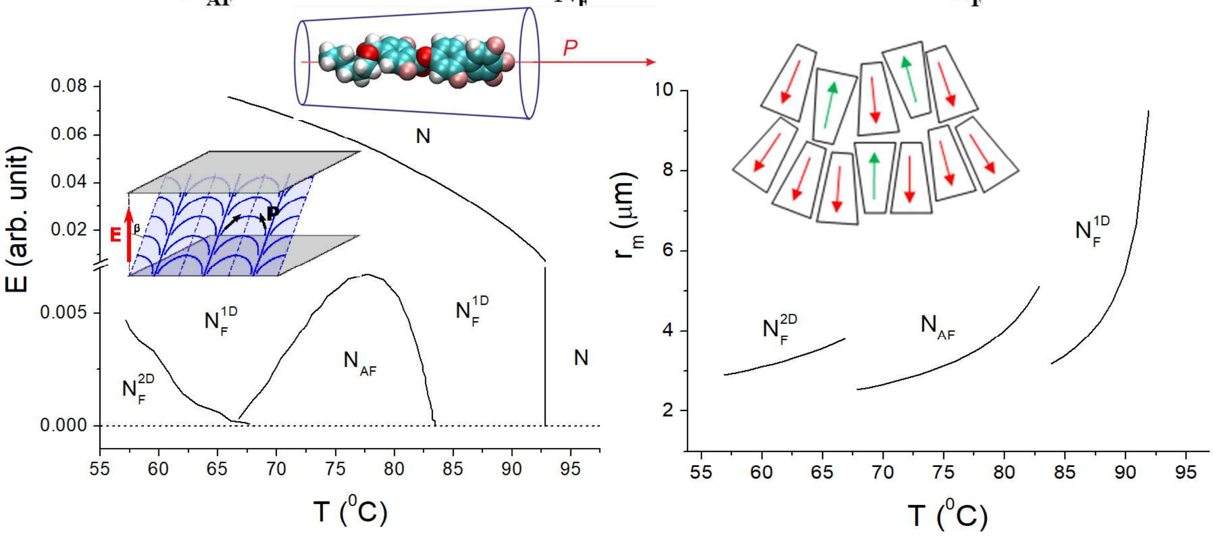
N_{AF}



N_F^{2D}



N_F^{1D}



The powerful technique of molecular-statistical physics has been applied for the description of structures and phase transitions in polar nematics induced by temperature variation and/or application of an electric field [1,2]. Three polar nematic phases were identified: the double-splay antiferroelectric nematic N_{AF}, the double-splay ferroelectric nematic N_F^{2D} and the single-splay ferroelectric nematic N_F^{1D} [images in the upper row]. In particular, the electric field – temperature phase diagram [lower row, on the left] and temperature dependence of the domain size in each phase [lower row, on the right] are obtained.

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Chiral domain states and electro-optics of ferroelectric nematic liquid crystals

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Keywords: Spontaneous chirality, periodic Frederiks transition, domain walls

A ferroelectric nematic liquid crystal is formed by achiral molecules with large dipole moments. Its three-dimensional orientational order is universally described as unidirectionally polar. Surface interactions align the spontaneous electric polarization of the ferroelectric nematic parallel to the substrates. We explore the electro-optic response of the ferroelectric nematic layers with different types of surface anchoring. We demonstrate that the ground state of a ferroelectric nematic unconstrained by externally imposed alignment directions is optically active, with left- and right-hand twists of polarization, Fig.1. Although the helicoidal deformations and defect walls separating domains of opposite handedness increase the elastic energy, the twists reduce the electrostatic energy and weaken when the material is doped with ions. An externally applied electric field unwinds the helices and produces complex three-dimensional structures. The study shows that the polar orientational order of molecules could trigger chirality in the soft matter with no chemically induced chiral centers.

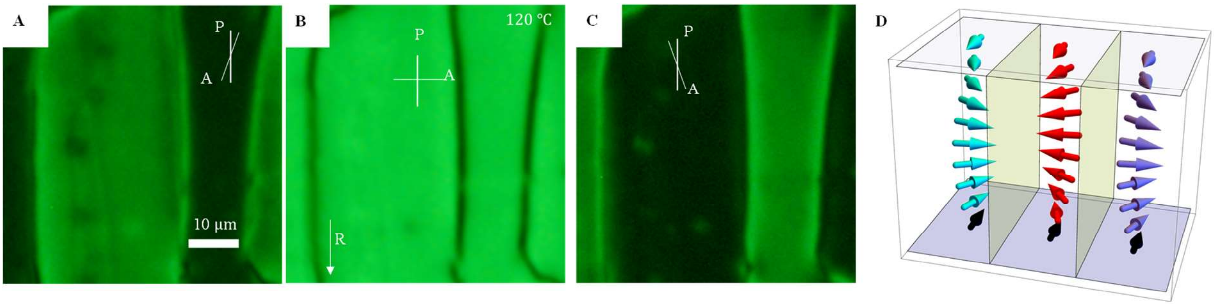

Figure 1: Chiral domains of a ferroelectric nematic with degenerate tangential anchoring at one surface: (A-C) polarizing microscopy textures, (D) polarization scheme of domains.

Acknowledgements: The work is supported by U.S. NSF grant ECCS-2122399, DMR-2215191, and DMS-2106675 by NASU via the project No. 0121U109816, and the Long-term program of support of the Ukrainian research teams at the Polish Academy of Sciences carried out in collaboration with the U.S. National Academy of Sciences with the financial support of external partners via the agreement No. PAN.BFB.S.BWZ.356.022.2023. The authors also acknowledge funding from the NATO SPS project G6030.

Director/layer dynamics of the smectic-Z_A phase in a ferroelectric nematic liquid crystal

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Keywords: Ferroelectric, nematic, dynamics, light scattering

The smectic-Z_A phase is among the more unusual mesophases in what has been called the "ferroelectric nematic realm" [1]. As a function of temperature, it occurs between nonpolar and ferroelectric nematic phases and exhibits a density wave running *normal* to the average molecular director. The smectic layers are planar ferroelectric slabs of ~9 nm thickness, stacked antiferroelectrically (i.e., with alternating planar polarization). We report on a dynamic light scattering study of the coupled director/layer dynamics of the smectic-Z_A phase in the compound DIO. The results are explained semi-quantitatively by the Hatwalne-Lubensky [2] elastic free energy theory of a tilted smectic specialized to the case of 90 degree tilt angle, provided certain features, such as a temperature-dependent chevron layer structure observed in cells of DIO with homogeneous planar anchoring [1], are accounted for. We give estimates of the elastic constants associated with the layer structure in the middle of the Z_A phase. We also compare the pretransitional behavior of viscoelastic parameters at the nematic to smectic-Z_A transition with behavior previously observed at a direct transition to the ferroelectric nematic phase in compounds such as RM734 [3].

Acknowledgements: Supported by US National Science Foundation under grant nos. DMR-221008 and ECCS-2122399.

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Diversity of chemical structures and physical properties of ferroelectric nematic liquid crystals

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Keywords: ferroelectric nematic, chemical structure, phase behavior, relaxor ferroelectric

Ferroelectric nematic liquid crystal (N_F LC) has attracted considerable attention for its unique viscoelastic nature, topology and electro-optical properties [1-4]. We have previously confirmed the ubiquitous existence of the N_F phase in rod-shaped molecules and established a general guideline for molecular design [5-6]. We found the most critical molecular parameter dictating N_F formation is the large enough dipole moment value, i.e. $\mu > 9$ D. Other factors including small geometrical aspect ratio of molecular shape and oblique dipole angle could help stabilize the N_F phase. In this presentation, we will show rather diverse chemical structure design exhibiting N_F phase, in both small molecules and polymers. Meanwhile, these N_F LCs with distinct chemical structures largely enrich the toolbox for tuning the physical properties of ferroelectric nematics, including SHG coefficient, dielectric permittivity, elasticity, viscosity, refractive anisotropy, phase transition pathway and temperatures. Finally, we will introduce our recent progress in the development of relaxor ferroelectric LC. Through the mixing of traditional non-polar N LC and emergent polar N_F LCs, a new type of liquid relaxor ferroelectrics is developed with continuous tunning of the ferroelectric domain size. Our work would definitely help push the future applications of N_F LCs in industry technology innovations.

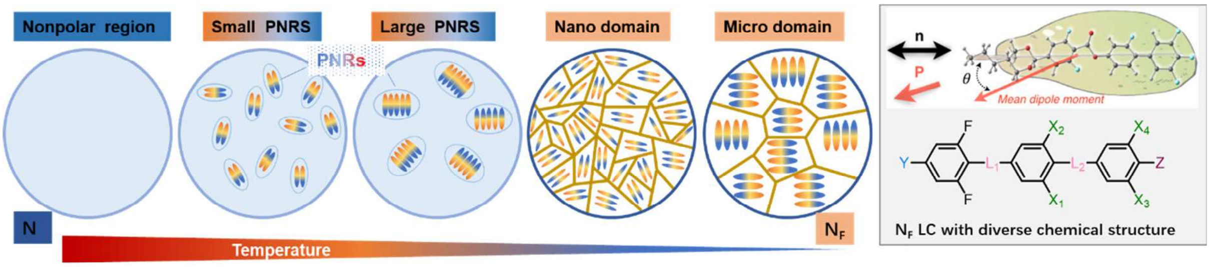

Figure 1: Diverse design of N_F LC chemical structures and the corresponding relaxor ferroelectrics.

Acknowledgements: M.H. acknowledges the supports from the National Key Research and Development Program of China (No. 2022YFA1405000), and the National Natural Science Foundation of China (NSFC No. 52273292).

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Drastic Hierarchical Reorganization from Ferroelectric Nematic to Helielectric SmecticC

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Keywords: structural color, ferroelectric nematic, helielectric smectic

Since the discovery of ferroelectric nematic (N_F) phase, the N_F liquid crystal (LC) has become the hottest topic in LC research and lead to discovery of several other phases. For example, helielectric phase (N_F*) was developed by mixing achiral N_F unit with chiral dopant or pure chiral N_F unit. On sharp contrast, the helielectric superstructure from pure achiral units is a big challenge. More recently, Karcz *et.al*[1] and Gibb *et.al*[2] separately reported in ArXiv preprints spontaneous formation of chiral helielectric superstructure of achiral units (compound **1**[1] and **2**[2]), resulting in structural reflective color. Compound **1** and **2** show the phase sequence N-N_x-N_F-N_{TBF}-SmC_F and N-SmA-SmA_F-SmC_P^H , respectively.

In this work, we developed novel enantiotropic ferroelectric materials exhibiting drastic phase sequence between N_F and helielectric SmC, in contrast to compound **1** and **2**. Rapid access to the compound was possible using mechanochemical synthesis.[5] The helielectric SmC phases also exhibit structural reflective colors (Fig. 1b). The structure and polarization behavior will be discussed in detail.

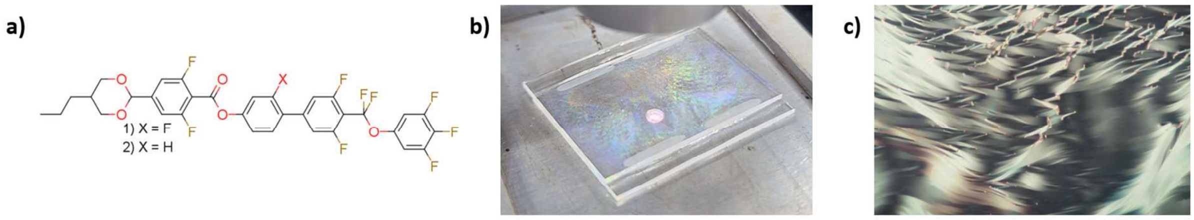

Figure 1: a) Molecular structure of previously reported **1** and **2.** Reflective color (b) and POM image (c) of helielectric SmC for our compound

Acknowledgements: JST (Japan Science and Technology) for funding *via* JST CREST

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Enantiotropic Ferro- and Antiferroelectric Nematic Phases in Cyano-Terminated and Fluorinated Phenyl Esters

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Keywords: ferroelectric, antiferroelectric, nematic,

We report mesomorphic, dielectric, and electro-optical properties and computational analysis of two cyano-terminated and fluorinated phenyl esters [1]. The presented materials show the enantiotropic nature and ferro- or antiferroelectric features of N_F and N_X nematic phases. The antiferroelectric behavior of the intermediate phase N_x was investigated using complementary methods, including differential scanning calorimetry, polarized optical microscopy, second harmonic generation (SHG), and dielectric spectroscopy. The SHG signal showed non-zero values in the N_F phase both on heating and cooling, which proves the enantiotropic character of this phase (Figure 1a). The compounds have a broad and low-temperature N_X phase, which permittivity dispersion is similar to the characteristics of DIO [2] (Figure 1b). A new model of collective and molecular relaxations considering the domain structure of the ferronematic phase is proposed [3].

The presented results will expand knowledge with new single-component compounds and multi-component mixtures with a very wide temperature range of the enantiotropic N_F and N_X nematic phase with significant application potential in the field of optoelectronics and photonics.

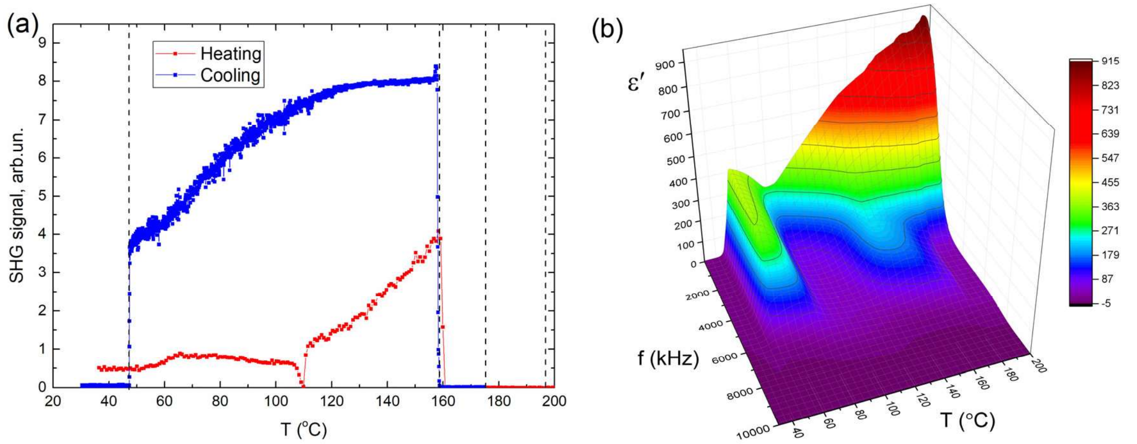

Figure 1: SHG signal (a) and dielectric spectroscopy results (b) of the compounds.

Acknowledgements: This work was supported by NCN project 2022/06/X/ST5/01316 and University project UGB 22-723

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Ferroelectric liquids on ferroelectric solids

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Keywords: (Ferroelectric nematic liquid crystals, polarization coupling, electromechanical instability, optical control of domain walls, lithium niobate)

In ferroelectric nematic (N_F) liquid crystals[1-4], where the polarization **P** is locally collinear to the optical axis **n**, polarized optical microscopy observations acquire the new meaning of an exploration of the electrostatic ground state of this phase, which is achieved in terms of the spatial arrangement of **P** at the micron scale. Indeed, in N_F, electrostatic interactions dominate over their fluid elasticity, so that the observed optical textures are mainly determined by long-range electrostatic forces and topological constrains. This lecture deals with a topological study on ferroelectric nematic droplets confined between two solid ferroelectric substrates. This investigation follows the recent observation of the electromechanical instability of sessile N_F droplets positioned on a bare lithium niobate ferroelectric crystal surface, exposed to either the pyroelectric[5] or photovoltaic[6,7] field. The additional friction from confinement and the smaller droplet volumes inherent to this geometry slows down the fluid motions with respect to sessile droplets, a feature that conveniently combines with the access to optical textures both in equilibrium and during the emission of fluid jets. Results indicate that the droplet texture and the shape of the polar domains are strongly affected by the tendency of N_F to minimize charge accumulation, in full agreement with the notion that the polarization field of this fluid phase can easily rotate to adopt configurations aimed at compensating any accumulation of electrostatic charge. The efficiency of this mechanism is particularly evident when the surface charging increases above threshold and gives rise to droplet instability.

Optical switching and reconfiguration of the domain walls that separate polar domains, will also be described and discussed. The findings could be helpful in designing optically controlled patterns of electric polarization and space charge.

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Ferroelectric nematic liquid crystals as electrocaloric materials

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Keywords: ferroelectric nematic liquid crystals, electrocaloric effect

The ferroelectric nematic (N_F) phase was first experimentally realized in 2017 in the liquid crystals (LCs) DIO, synthesized by Nishikawa et al. [1], and RM734, synthesized by Mandle et al. [2,3] It quickly became apparent that the phase had unique properties that could be geared towards a variety of applications including: large dipole moment; giant values of spontaneous polarization in comparison with other ferroelectric liquid crystal phases such as the chiral smectic-C (SmC*) phase; large phototunable dielectric permittivity and nonlinear optic coefficients, among others. [4-7] Justifiably, the phase has become a 'hot topic' in the field of liquid crystalline research.

Most commonly, liquid crystals find use in electro-optic applications but as highly polar fluids there is potential for N_F materials in other areas, for instance in energy applications as electrocaloric (EC) materials. The electrocaloric effect refers to a change in the temperature of a material when an electric field is applied or removed. Existing EC device concepts utilize solid state or polymeric ferroelectrics as the EC material along with a heat-exchanging fluid; it has been previously suggested by Tipping et al. [8] that the ferroelectric liquid crystalline SmC* phase, with an EC temperature change of 0.37K, might be considered as both EC material and the heat-exchanging fluid, though the achievable temperature change is too small in such materials because of their relatively small spontaneous polarisation. This logic is extended to the N_F phase, which has comparable ferroelectric coefficients to solid ferroelectrics and thus is more likely to achieve an electrocaloric response sufficient for technological applications.

Here, the electrocaloric behavior of several N_F materials is presented, and a comparison is made with ferroelectric ceramics and polymers, demonstrating their enormous potential.

Acknowledgements: The authors acknowledge funding from ESPRC and Merck Electronics KGaA. We also acknowledge the supply of materials from Merck Electronics KGaA.

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Ferroelectric nematics based on dimethylamino terminated part: textures and defects

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Keywords: nematic, ferroelectricity, polar nematics

Since the recent discoveries, ferroelectric nematic phase, N_F, has become of upmost interest [1,2]. The ongoing research has been concentrated on the design of new molecular structures and intensive investigations of their physical properties are carried out. Recently, we designed and studied a new molecular structure [3] terminated by dimethylamino group, and we observed the N_F phase on cooling from the isotropic phase. For several homologues, the N_F phase is stable and persists down to the room temperatures.

In this contribution, we will report on the polarized microscopy textures observed in various geometries and for different electric field direction. Among others, we will describe the textures in the homogeneous cell with antiparallel alignment. In such a cell, the molecules are mainly arranged in twisted domains with borderlines oriented preferentially perpendicular to the surface alignment (rubbing direction). We will describe these domains and present a model of 2π disclinations, which are separating the areas with an opposite twist sense. In Figure 1, we demonstrate the annihilation of a small segment with opposite twist in a planar 5 μm cell with antiparallel rubbing directions at opposite glass surfaces.

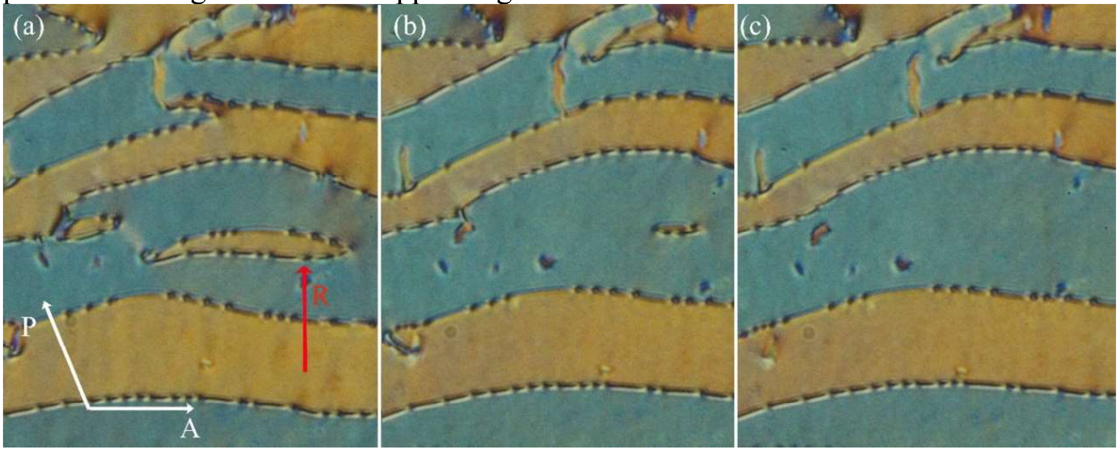

Figure 1: Planar textures in a 5μm HG antiparallel cell shows twisted domains with slightly uncrossed polarizers: (a) at a starting time t=0, (b) after 10s, and (c) the situation after 20 seconds. A red arrow marks the rubbing direction.

Acknowledgements: Authors acknowledge project MAGNELIQ, the European Union's Horizon 2020 research and innovation programme, grant agreement No 899285.

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Ferroelectric Nematics: Electric Field Guiding and Polarization Control

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Keywords: Ferroelectric Nematic, Microchannel, Polarization, Field guide

Among the unique properties of ferroelectric nematic liquid crystalline phase (N_F) is their response to external electric field **E**, resulting from the combination of large spontaneous polarization and fluidity. We find that the confinement of N_F in microchannels terminating at electrodes is an effective way to enlighten a variety of distinctive features of such responsiveness.

We first considered channels that connect two terminal electrodes via straight and curved path which we filled with the N_F mesogen RM734. When low DC electric fields (**E** ≥ 0.5 V/mm) are applied to the N_F phase, the polarization **P** smoothly aligns along the channels, even in sections oriented perpendicular or opposite to the line connecting the electrodes. Analysis of the switching process following **E** reversal demonstrates that the electric field in the channels is uniform and oriented along their axes, an effect of the ability of N_F to rapidly accumulate significant amounts of bulk and surface charge through minuscule collective orientations[1].

The study of bifurcated channels, in which the channel shape would favor a specific splay geometry respond differently to positive vs. negative voltage drops, a consequence of the broken symmetries inherent to the polar ordering of N_F.

Finally, the study of channels connecting multiple electrodes enables the characterization of the propagation of **E** when bifurcations are present. Thee controlled distribution of **E** allows to modulate **P** and scattering state of different sections in arrays of microchannels.

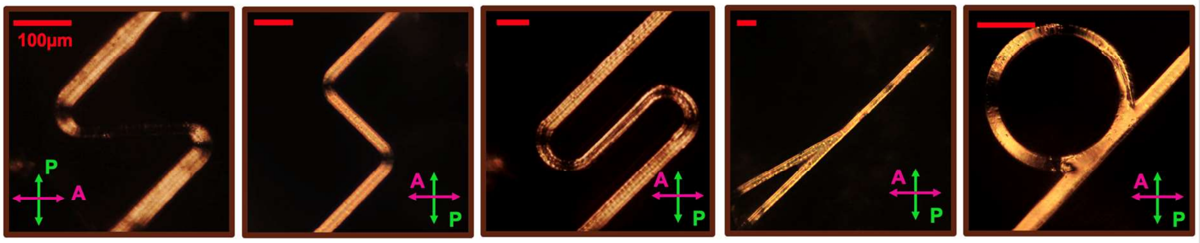

Figure 1: Polarized Ooptical microscopy images of microchannels filled with RM734

Acknowledgements: Petra Paiè and Roberto Osellame (Istituto di Fotonica e Nanotecnologie, Consiglio Nazionale delle Ricerche, Milano, Italy) for producing microchannels.

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Giant Permittivity in Super Dielectric Liquids

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Keywords: ferroelectric nematic liquid crystals, permittivity, dielectrics.

The long-awaited ferroelectric nematic LCs (NF) predicted more than a century ago were finally discovered in 2017, independently in two different materials: RM 734 [1] and DIO [2]. The two common features of these materials are (a) extremely high molecular dipole moment (μ ~10 D) and (b) giant dielectric permittivity (ε′ ~ 10,000) in the ferroelectric nematic phase. Two new compounds, WJ-16 and WJ-18, based on the chemical structure of DIO, were synthesized for a further enhancement of ferroelectricity by increasing the molecular dipole. As expected, both compounds exhibit extremely high dipole moments (10.6 D and 13.6 D respectively). However, unlike DIO, giant permittivity was observed not only in the ferroelectric nematic phase, but it was also in the SmA and even isotropic (!) phases (see Fig.1) which is obviously non-ferroelectric. After intensive study it is concluded that both samples are paraelectric rather than ferroelectric and they belong to the class of super-paraelectrics (SPE) observed before in the solid state and here for the first time in liquid phases. As this is the first known example of a superparaelectric liquid, it opens a new range of applications of liquid crystals as the working media for supercapacitors with the potential of using them in energy storage devices.

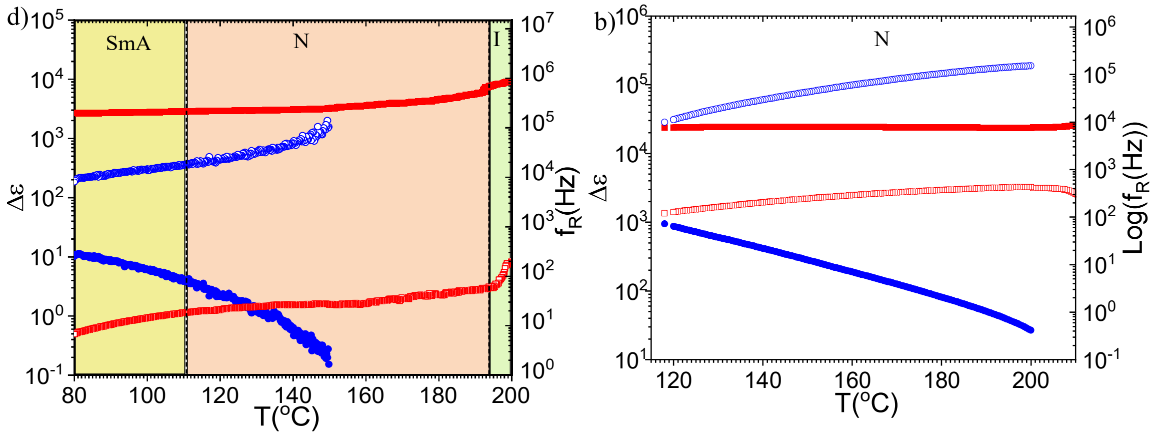

Figure 1: C) Temperature dependence of the dielectric strength (filled) and frequency (open) in a 4 μm uncoated (no alignment layers) cells of (a) WJ-16 and (b) WJ-18.

Acknowledgements: We thank the Irish Research Council for awarding the Government of Ireland PDF 2021, GOIPD/2021/858; and the CSC, China for a PhD scholarship.

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Interfacial instabilities in ferroelectric nematics exposed to electric fields

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Keywords: pattern formation, ramification, labyrinth, fractal growth

The combination of huge spontaneous electric polarization with three-dimensional fluidity is a unique feature of the novel ferroelectric nematic liquid crystals. Polar characteristics and flow properties described by low viscosities are also observed in magnetic ferrofluids, in which we can see various magnetic field induced spectacular interfacial patterns, spiky structures as consequences of instabilities named after Rosensweig [1]. Based on the analogy between magnetism and electricity, we can expect interfacial instabilities also in ferroelectric fluids exposed to electric fields. We present that in ferroelectric nematics, more, distinct types of electric field induced interfacial instabilities can be observed, depending on the geometry, and the properties of the applied electric field, such as magnitude and frequency. The primary pattern forming mechanism called ramification [2] exhibits a sharp threshold voltage and results in stationary fractal-like fluid structures tunable by voltage above the threshold as seen in Figure 1. At higher voltages, a clearly distinguishable secondary instability occurs and the resulting morphology resembles a labyrinth. Our experimental results, supported by finite element method simulations, show the crucial role of the unexpected structure of the electric field depending on the geometry.

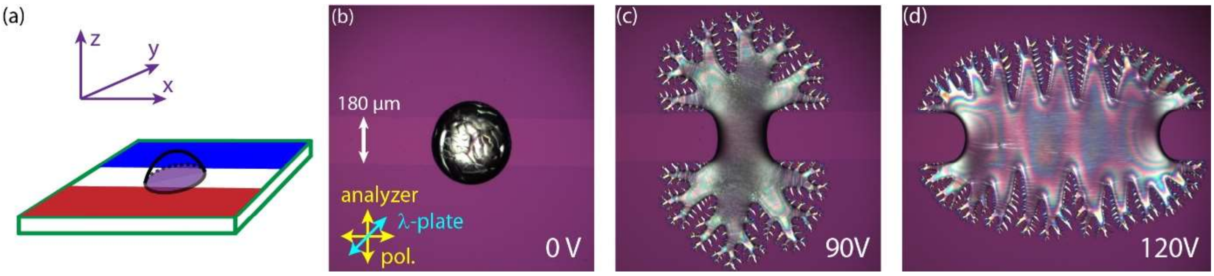

Figure 1: Emergence of the primary, ramification instability in a ferroelectric nematic sessile droplet exposed to electric fields

Acknowledgements: This work was supported by the projects NSF DMR 2210083, NKFIH FK142643 and 2023-1.2.1-ERA_NET-2023-00008.

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Mechanochemical-Assisted Screening of Ferroelectric Fluid Molecules

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Keywords: ferroelectric nematic, mechanochemistry

Recently, the mechanochemistry (MC) revives attention as a technology for organic synthesis. The MC-assisted reaction offers a sustainable alternative to conventional solution-chemical synthesis because of easy setup, fast reaction, solvent-minimized/-free systems, high selectivity, better controllability, and less chemical waste. Furthermore, the MC reactivity is easily controlled because the collision factor A in the Arrhenius' equation, $k = A\exp(-E_a/RT)$, depends on the mechanical frequency of mixing. So far, in materials science, the MC synthesis has been employed for the development of various functional molecules, such as dyes, emissive molecular semiconductors as well as polymers [1]. In theory, the molecules exhibiting LC phases can be also created via multi-step MC synthesis by linking multiple chemical building blocks one-by-one. If the starting blocks with a high permanent dipole moment (μ) are selected so that the overall μ after series liking becomes > 8.5 Debye, it is most likely to generate the ferroelectric fluids (FF) exhibiting ferroelectric nematic [2,3], ferroelectric smectic LC phases [4,5] (Fig.1), which have been becoming a hot topic in the field of LC physics/chemistry from fundamental science and application aspects. In this presentation, we will discuss the high-throughput screening of FF molecules using the MC synthesis. This strategy may be suitable for obtaining optimal molecular parameters, which are required in materials informatics.

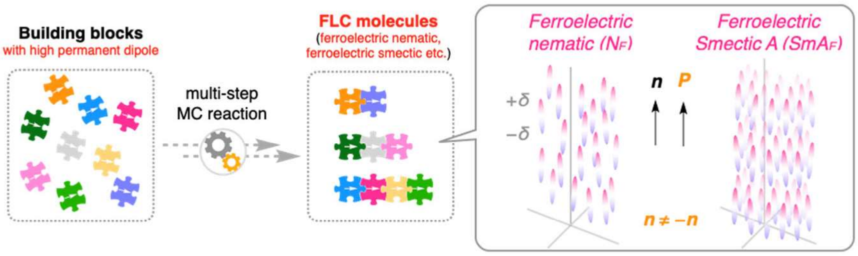

Figure 1: Multi-step MC screening of FF molecules.

Acknowledgements:

This work was supported by JSPS KAKENHI Grant Numbers (JP22K14594; HN, JP21H01801; FA), RIKEN Special Postdoctoral Researchers (SPDR) fellowship (HN), FY2022 RIKEN Incentive Research Projects (HN), and JST CREST (JPMJCR17N1; FA) and JST SICORP EIG CONCERT-Japan (JPMJSC22C3; FA).

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Molecular-statistical approaches to ferroelectric nematics

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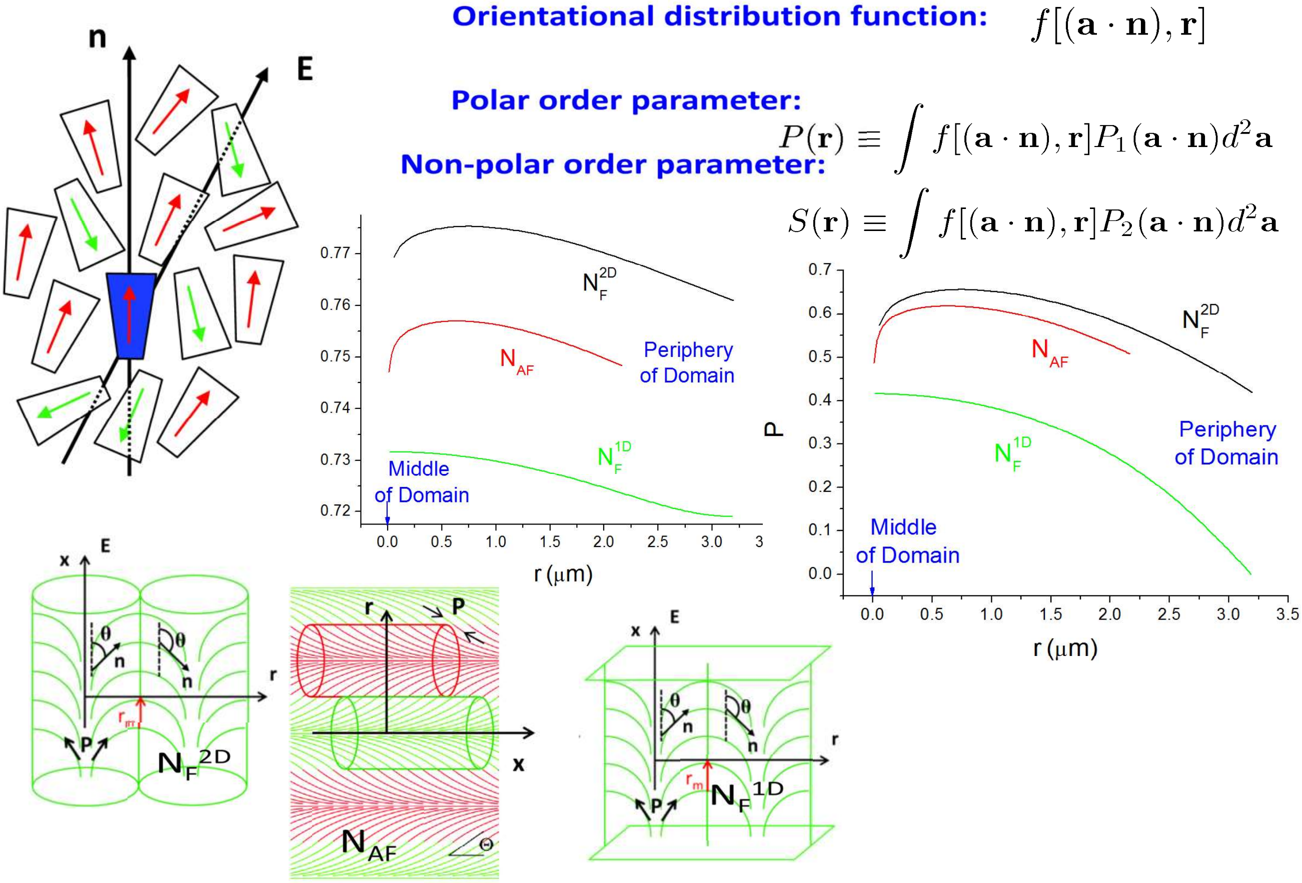
Keywords: ferroelectric and antiferroelectric nematics, splay phases



The structures of several polar nematic phases are obtained in the framework of molecular-statistical approach. Distributions of the director, polar and non-polar order parameters within the domain of each phase are found. It is demonstrated how the thermal fluctuations can select between various symmetries and trigger the phase transitions [1,2].

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New RM734-like Fluid Ferroelectrics Enabled through a Simplified Protecting Group Free Synthesis

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Keywords: Ferroelectric Nematic (N_F) phase, Organic synthesis, DFT, MD simulations.

In 2017, Mandle et al. [1] and Nishikawa et al. [2] simultaneously and independently reported highly polar liquid crystalline materials that exhibited multiple nematic phases. The lower temperature nematic phase is now understood to be polar, now termed the ferroelectric nematic (N_F) phase, and is currently the focus of considerable research. The most widely studied compound which exhibits the N_F phase is RM734. Typically, this is synthesised left-to-right, installing the 4-nitrophenyl unit last and employing a benzyl protecting strategy. The benzyl group enables high yields, but the hydrogenolysis deprotecting step brings issues of functional group compatibility limiting the chemical diversity of resulting materials.

We report a novel simplified synthetic procedure for making analogues of the widely studied ferroelectric nematogen RM734 (Figure 1) [3]. Our new procedure focuses on building materials starting from the nitro-terminus and eschewing protecting groups, in contrast to previously reported syntheses [4,5]. This new synthetic approach confers two principal advantages; firstly, the synthesis of the variants described herein is expedient, being a single step as opposed to three or more via the classical route. Secondly, by forgoing the use of benzyl groups as utilised in the original synthesis we can include functionality that is incompatible with hydrogenolysis conditions (e.g. olefins, late halogens, unsaturated heterocycles). We report several RM 734-like materials which exhibit the N_F phase and we rationalise this behaviour with aid of electronic structure calculations, potential energy surface scans and atomistic molecular dynamics simulations.

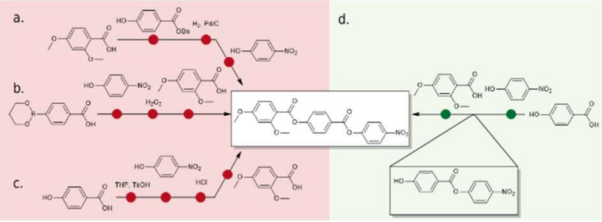

Figure 1: (a) Original synthesis of RM734 reported by Mandle et al. [1] , (b-c) alternative synthetic routes proposed in other work [4, 5], and (d) synthetic route developed and used in this work [3].

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Order-disorder Ferroelectric behavior in N_F materials as probed by Raman spectroscopy

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Keywords: polar order, order-disorder, polarized Raman spectroscopy, order parameters.

In 2017, the ferroelectric nematic phase (**N_F**) was observed, more than a century after it was first theoretically predicted. [1-3] The ferroelectric nematic phase exhibits polar ordering $\hat{n} \neq \hat{n}$ where $\hat{n}$ is the nematic director, in contrast to the ordinary nematic phase (N), which is apolar. The fundamental interest in the **N_F** phase as a polar, ordered fluid system is enhanced by the reports of these materials exceptionally large dielectric permittivities and spontaneous polarization values. [3] As such ferroelectric nematic are expected to have far-reaching applications in non-linear optic devices, fluid capacitors for energy storage and photonic devices. [3-4] For these reasons, in addition to the fundamental interest in understanding the behaviour of a polar nematic fluid, it is of utmost importance to understand the order parameters within the phase.

In this talk, we report the uniaxial order parameters of RM734, one of the first examples of the ferroelectric nematic phase, as determined via Raman spectroscopy and birefringence measurements. The findings are interpreted by drawing parallels between the ferroelectric nematic fluid phase and solid-state ferroelectric materials. It is suggested that the existence of polar order, and/or a change in the reorientational dynamics of the molecules, at the onset of the **N_F** phase may be reflected in the changes in the full-width half maxima of the Raman signal. The energetic barrier of the transition from the para-electric to ferro-electric phase is found to be of the order of 2.5±0.6 kJ/mol, which is considerably lower than the energetic barrier in solid ferroelectric materials.

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Origin of ferroelectric ordering in nematic liquid crystals, long range interactions and electrostatic properties of ferroelectric materials.

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Keywords: ferroelectricity, nematics, long range interactions, thermodynamic potentials.

The possibility of ferroelectric ordering in nematic liquid crystals has been discussed for decades using simple models of hard and soft anisometric particles with large dipole moments [1]. Recently the ferroelectric ordering has indeed been discovered [2-5] in few nematic materials with rather complex molecular structure which includes several dipoles and polar charge distribution along the molecular surface [6]. We discuss in detail the possible molecular origin of ferroelectricity in the nematic phase considering a number of models based on direct dipole-dipole interaction, electrostatic interaction between surface charge densities and the model which combines dipole-dipole interaction and short-range orientational-translational correlations. In particular we derive a contribution to the total free energy of the long-range tail of the dipole-dipole interaction potential and show that this contribution depends on the sample shape and on the boundary conditions [7]. As a result this shape dependent contribution may strongly effect the transition into the ferroelectric phase depending on the actual boundary conditions maintained experimentally.

We also consider two conjugated thermodynamic potentials which depend on the electric field in the medium and on the displacement field, respectively. The actual polarization in the nematic medium corresponds to the minimum of one of these potentials depending on the boundary conditions which may have significant experimental consequences. In the framework of the general Landau de Gennes theory, which employs both potentials, we discuss in detail the ferroelectric properties of different nematic cells including the ones with fixed applied voltage, free cells with disconnected electrodes and cells with fixed charge density at the electrodes.

Acknowledgements: I am grateful to Mark Wilson, Epifanio Virga and Alberta Ferrarini for many interesting discussions.

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Polar alignment states of a ferroelectric nematic on obliquely evaporated surface layers.

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Keywords: (ferroelectric nematics, polar alignment, oblique evaporation)

Ferroelectric nematics [1-4], may enable new types of technological applications in which the boundary conditions will play a crucial role for their function. It has been shown that conventional, rubbed polyimide layers provide polar in-plane anchoring of the ferroelectric nematic (N_F) phase [5,6]. Here we demonstrate that surfaces coated with obliquely evaporated SiO_2 layers facilitate two stable polar surface anchoring states of the ferroelectric nematic RM734, with azimuthal orientations $\pm \phi$ controlled by the evaporation angle α. The two-fold polar alignment was observed and demonstrated in sample cells combining a SiO_2 coated substrate with a circularly rubbed polyimide-coated surface (ECR cell), cf. Fig.1.
Two-fold alignment on obliquely evaporated surface layers is known for conventional non-polar nematics [7,8]. We suggest that in the case of ferroelectric nematics the polar two-fold alignment might be further explored e.g. for bistable ferroelectric nematic devices.

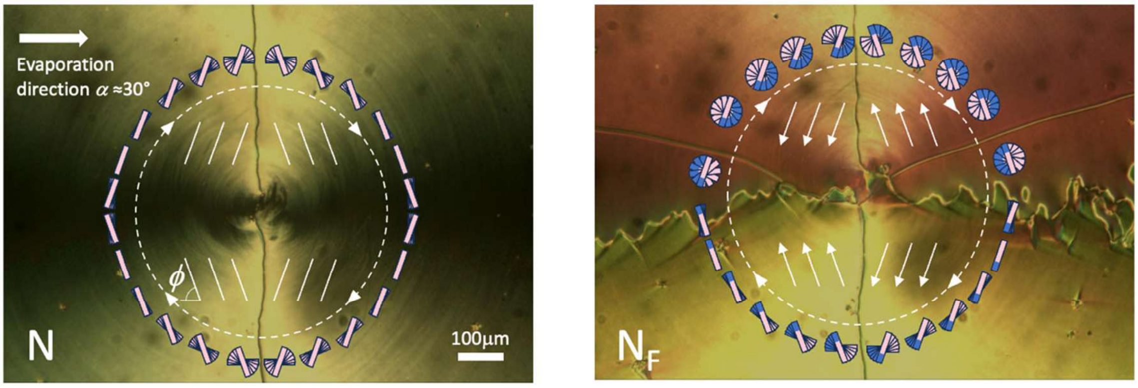

Figure 1: 4µm thick ECR cell filled with RM734; circular rubbing on the lower (-----) and SiO_2 (α ~30°) on the upper substrate. The surface alignment on the SiO_2 surface is indicated with solid lines (N left) and arrows (N_F right), respectively. The up-down asymmetry in the N_F case demonstrates the in-plane polarity of the surface states in N_F.

Acknowledgements: Part of this work was financed by the Swedish Research Council.

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Polarization Direction Configuration of Ferroelectric Nematic Liquid Crystals on the Surface of Alignment Films

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Keywords: ferroelectric nematic liquid crystals, alignment treatment, polarization direction

Ferroelectric nematic liquid crystals (NFLCs) are expected to have novel applications based on their ferroelectric properties and unique phenomena [1]. For device applications utilizing their properties, it is necessary to control the polarization domain by alignment control. The polarization state on the substrate surface of NFLCs and the effect of orientation treatment on them have been studied [2]. In our previous study, in rubbed polyimide films, the positive side of the NFLC polarization direction is uniformly fixed on the substrate surface [3], but the general orientation mechanism has not yet been clarified. Here we investigate the effects of pretilt and alignment film polarity, parameters on the substrate surface applied by the alignment treatment, on the polarization state of the NFLC surface.

We prepared cells with pretilt, by rubbing polyimide alignment film and oblique light irradiation of azo-based photo-alignment film, and cells without pre-tilt, by not rubbing and normally irradiating linear polarized light. As a result, we found that in the case with pretilt, the polarization direction is uniformly fixed on the substrate surface as in the previous study with rubbing treatment [3], while in the case without pretilt, the polarization direction is not uniformly fixed on the substrate surface. In other words, it is determined whether the polarization direction on the substrate surface is uniformly fixed or not by the presence or absence of pretilt. In addition, it is known that the rubbing treatment has an electrical effect with pretilt, but we found this electrical effect has almost no effect on the polarization state on the substrate surface.

We also investigated the effect of alignment film polarity by fabricating anisotropic hybrid cells rubbed with homeotropic alignment films of different polarity, and performed optical simulations and observed the electric field response. In our previous study, we found that the positive side of the polarization direction is uniformly fixed on the substrate surface for polyimide alignment film [3], but in this study, we found that the polarization direction uniformly fixed on the substrate surface changes depending on the alignment film polarity. As an application of these results, we demonstrated uniform out-of-plane orientation of NFLCs.

Acknowledgements: This work was partly supported by MEXT KAKENHI (JP21K18722, and JP23H02038), and the Grant-in-Aid for Scientific Research (A) JSPS KAKENHI Grant Nos. JP23H00303 from the Japan Society for the Promotion of Science (JSPS). Partial components of the liquid crystal mixture were provided by JNC Petrochemical Corporation.

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Polarization patterns of ferroelectric nematics not constrained by polar surface interactions

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Keywords: Splay and twist deformations, photoalignment, domains.

Surface interactions play an important role in aligning liquid crystals. The recently discovered ferroelectric nematic (NF) shows a uniform monocrystal orientation of spontaneous electric polarization when confined between two plates with unidirectionally treated substrates. We explore NF structures in which the surface conditions are less restrictive and produce either bidirectional apolar or azimuthally degenerate alignment at the bounding plates. The bidirectional apolar alignment with a prepatterned +1 radial defect is achieved by photoalignment. The radial structure splits into domains of splay and twist deformations, in which the polarization alternates between being inward and outward directed. In the case of azimuthally degenerate confinement at one plate, the texture splits into domains with an alternating sense of twist. Both patterns form to reduce the electrostatic energy associated with the unidirectional orientation of electric polarization. The study demonstrates a dramatic difference between the domain structures in solid ferroelectrics, in which the polarization follows the crystallographic axes, and liquid ferroelectrics, in which the absence of these axes allows the polarization field to deform smoothly in response to the boundary conditions and the electrostatic energy minimization.

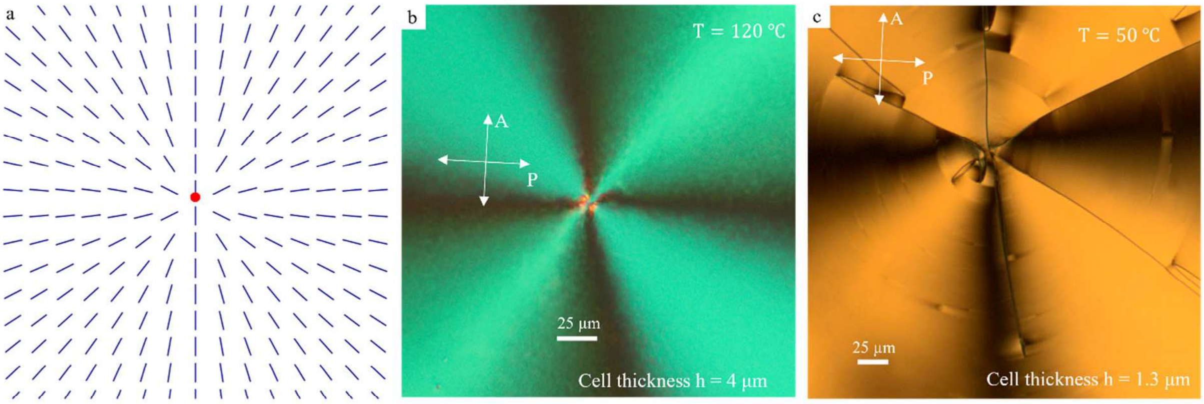

Figure 1: Photo-patterned surface alignment of an NF material on +1 radial defect pattern: (a) Radial defect pattern used in the alignment (b) N texture of DIO where director follows the surface pattern (c) DIO texture in NF phase exhibiting alternation of polarization vector **P** inward and outward.

Acknowledgements: The work is supported by U.S. NSF grant ECCS-2122399.

Polarization topology of polar nematic fluids in confinement

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Keywords: ferroelectric nematic, helielectric nematic, topology, confinement

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

The emerging new class of materials, dubbed ferroelectric nematic states [1-5], exhibits the head-to-tail asymmetry. In this presentation, we will discuss several exciting polarization topological structures using either the achiral or chiral ferroelectric nematic liquid crystals in confined space (e.g., Fig. 1). We will show that the flexoelectric and depolarization field effects that compete with the traditional nematic elasticity play crucial roles in dictating the deformation of polarization textures.

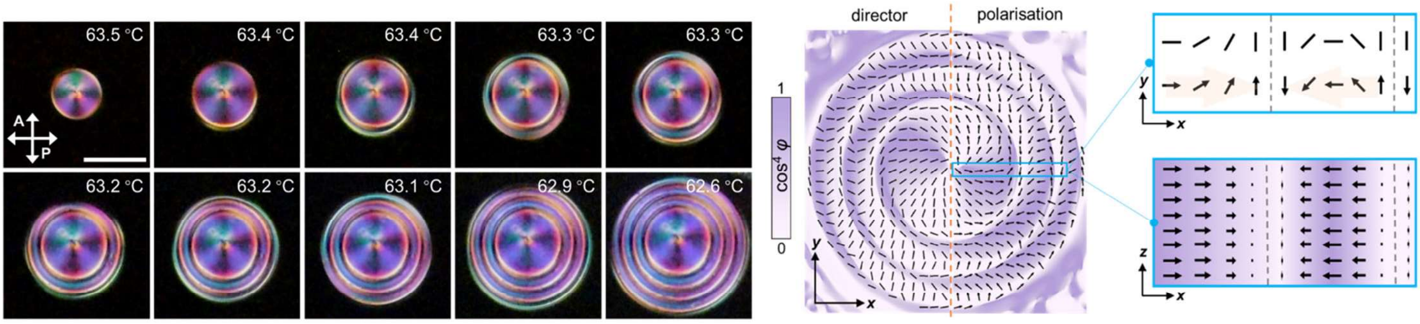

Figure 1: Toroidal polarization topology in helielectric nematic droplets.

Acknowledgements: S.A. acknowledges the supports from the National Key Research and Development Program of China (No. 2022YFA1405000), the Research Fund for International Excellent Young Scientists (RFIS-II; No. 1231101194) and the International Science and Technology Cooperation Program of Guangdong province (No. 2022A0505050006).

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Room-Temperature Ferroelectric Nematic Liquid Crystal Showing a Large and Diverging Density

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Keywords: Ferroelectric nematic, liquid crystal, density

The ferroelectric nematic phase (N_F) is a recently discovered liquid crystal mesophase characterized by the coupling of orientational order and polar order [1-4]. Atomistic simulations indicate that the polar N_F phase may exhibit higher density compared to conventional nematics due to contributions from polar ordering [5]. Employing an oscillating U-tube densitometer, we acquired detailed temperature-dependent density values for the room-temperature nematic, M5 [6]. We support this result with density measurements of a series of conventional liquid crystals, which have excellent agreement with previous findings. We present the first experimental density data for a N_F material, in addition to a nematic not previously reported, CCU-3-F. M5 exhibits a consistently high density (>1.3 g/cm^3) at all temperatures studied, even in phases lacking polar order. Density increases were observed on cooling through phase transitions, with the intermediate-to-ferroelectric nematic (N_X-N_F) transition displaying an order of magnitude smaller increase compared to the isotropic-nematic (I-N) transition.

To further explore the implications of M5's density, we measured its refractive indices (n_o and n_e) and compared the average refractive index, n_{avg} with those of 5CB and polar smectic liquid crystals. The highly polar nature of the system was found to counteract the effects of a larger density. Guided by the assumption of a high density for NF materials, we derived an approximation enabling the determination of the polar order parameter, ⟨P1⟩, from polarization measurements.

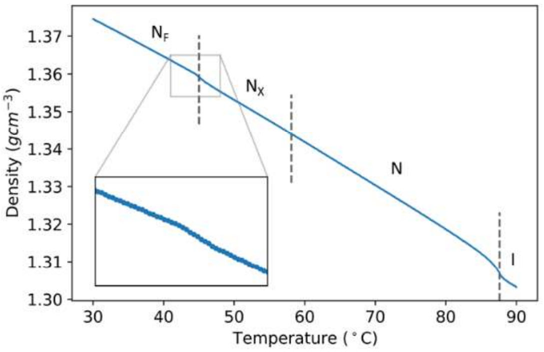

Figure 1: Temperature-dependent density behaviour for the NF

Acknowledgements: The authors thank Merck Electronics KGaA for gifting the sample of M5 used in this work, and for their continued partnership and support. HFG thanks EPSRC for funding via grant number EP/V054724/1. RJM thanks UKRI for funding via a Future Leaders Fellowship, grant number MR/W006391/1, and UoL for funding a PhD studentship for CPB.

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Stability and Dynamics of Ferroelectric Nematics: Charge and Molecular shape in Atomistic Simulations

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Keywords: Ferroelectric Nematic, Atomistic Simulations, Molecular Dynamics

The historical search for a liquid-crystalline phase with global polar order made significant advances when Nishikawa et al. [1] and Mandle et al. [2] independently discovered the ferroelectric nematic phase, characterized by novel, lightweight rodlike molecules, DIO and RM734. This phase is distinguished by its high dielectric permittivity, nonlinear electro-optical properties, and fluidity, positioning it as a promising alternative for technological applications, surpassing traditional ferroelectric solids.

Although Li et al. [3] have thoroughly investigated some molecular aspects necessary for the ferroelectric phase's stabilization, large longitudinal dipole moments and polarizability are not the only factors influencing the formation of a long-range polar order in nematic phases. As Berardi et al. [4] showed, pear-shaped mesogens with unequal head-tail interactions can result in a globally polar nematic phase. Our objective is to understand the mechanism behind the phase transition to a long-range polar nematic state, focusing on whether it's driven by dipole-dipole electrostatic interactions or the molecules' tapered shape.

In this study a comprehensive atomistic simulation of charged and chargeless topologies of DIO molecules within the ferroelectric nematic phase was investigated. The spatial and orientational correlation distribution function and dynamics were analyzed. For charged DIO topologies, the research reveals a favorable alignment of head-to-tail and parallel side-by-side arrangement of molecules, which adopt a correlated orientation conducive to polar ordering. On the other hand, chargeless topologies of DIO molecules show no polar ordering, with antiparallel alignment between molecules. Understanding these mechanisms is crucial for harnessing this novel phase in advanced technological applications and devices.

Acknowledgements: de Mello, M. acknowledges financial support from The Japanese Ministry of Education, Culture, Sports, Science and Technology (MEXT), The Graduate School of Science of Kyoto University, and the GINPU Fund Grant. Araki, T. acknowledges the JST CREST Grant Number JPMJCR2095 and JSPS KAKENHI Grant Number 21K03486.

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The Structure of the Ferroelectric Nematic Phase: Insights from Molecular Dynamics Simulations

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Keywords: Ferroelectric Nematic, Atomistic Simulations, Molecular Dynamics

The reported experimental discovery of a ferroelectric nematic (N_F) phase is an exciting new development in liquid crystal research. [1-3] The new phase has several potential applications in displays and novel technology due to its unprecedented polarization. However, the origins of the phase are poorly understood, leading to derivatives of the first two mesogens to be discovered making up most of the known N_F mesogens.[1] At a molecular level, the phase is unusual, as often molecules with large dipole moments preferentially align with anti-parallel dipole ordering, as seen (for example) in cyanobiphenyl-based nematics, such as 5CB. However, in the N_F phase, large molecular dipoles preferentially align in a parallel direction.

Here, we report state-of-the-art atomistic molecular dynamics simulations of an N_F mesogen: "DIO-F" (Fig. 1). We initially use quantum chemical calculations to optimise a new force field for DIO-F, and from molecular dynamics simulations of up to 648 molecules, we obtain excellent predictions of phase properties and transition temperatures. The N_F phase is obtained by cooling an isotropic phase and allowing the N_F phase to grow slowly over hundreds of nanoseconds of simulation. Cylindrical distribution functions are calculated to investigate the role of specific preferred intermolecular pairings. The calculations allow different explanations for the stability of the N_F phase to be probed.

N_F stability is found to be promoted by a combination of local quadrupolar interactions and microphase separation of hydrophobic parts of the molecule. These interactions are sufficient to overcome the tendency for anti-parallel dipole alignment that is seen in many low molecular weight nematic and smectic systems.

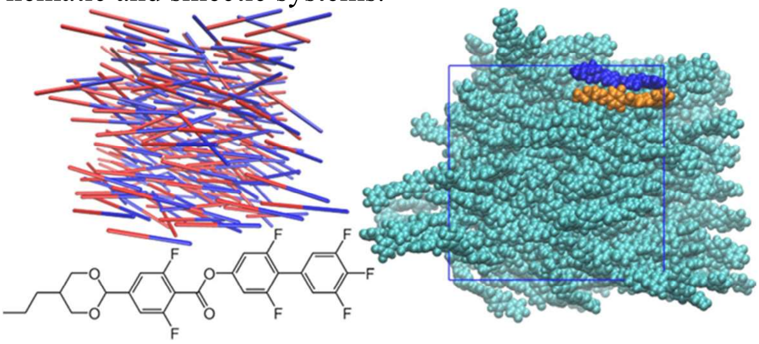

Figure 1: Visualisation of a ferroelectric nematic phase of "DIO-F ".

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Three New Chemical Structure Spaces Exhibiting the Ferroelectric (N_F) Nematic Phase.

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Keywords: Ferroelectric Nematic (N_F) phase, Organic synthesis, Structure-property relationships.

Since the practical discovery of the ferroelectric nematic (N_F) phase at equilibrium in the late 2010's, the phase has garnered significant excitement prompting it to be studied extensively as it has been 'promised to remake nematic science and technology' [1]. Despite the work which has been carried out to date, studies into the N_F phase are still in their infancy. The current materials being studied are all based on 3 archetypal structures: RM734 [2], DIO [3] and UUQU-4N [4]. These current materials present the unwelcome combination of challenging working temperature ranges and often low chemical stability. This has driven a significant appetite for new materials that can sustain the polar mesophase at and below ambient temperatures [5][6].

We report the synthesis and liquid crystal characterisation of some 150 new, highly fluorinated compounds based on three novel structure types. Of the 150 materials studied, some 50 of these materials are ferroelectric nematogens – the largest single study into the chemistry of the N_F reported to date. Although some of these compounds melt and exhibit the N_F phase close to ambient temperature (circa 40 ºC), we achieve true room temperature example of the phase through the formulation of binary mixtures. Due to the novel structures reported, these mixtures are more chemically stable than previously reported mixtures, stabilising the N_F phase over large temperature ranges.

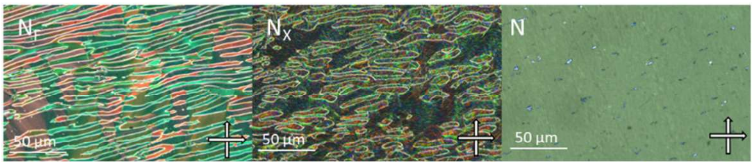

Figure 1: POM micrographs depicting the phase profile of one of the ferroelectrics nematogens reported in this study. Images are taken within 9.5 µm cells treated for a planar anchoring condition.

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Towards heliconical ferroelectric nematic phase – molecular design history

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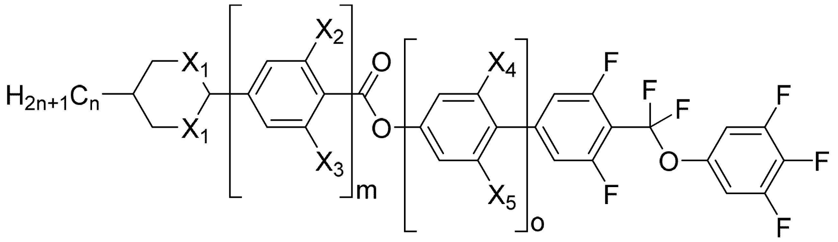
Keywords: heliconical, ferroelectric, nematic, polar, synthesis

Polar LC materials have become the center of interest for scientists as they were found to exhibit polar nematic phases e.g. ferroelectric (N_F) and antiferroelectric (N_X) phases. Since the experimental confirmation[1] of the theoretically predicted ferroelectric nematic phase, there has been extensive research on the development of novel polar materials exhibiting desired LC properties. Recently, we have reported the very first example of a compound with an enantiotropic ferroelectric nematic phase, whose molecular structure was based on DIO[2]. Further modification of the chemical structure led to the discovery of a new chiral LC phase in which polar order occurs together with the spontaneous formation of the helical structure built from achiral molecules[3].

Here we demonstrate how the molecular structure of new polar materials affects their mesomorphic properties. Compounds designed specifically for exhibiting heliconical ferroelectric nematic phase have their phase sequences highly sensitive to small changes in their structure, however most of them exhibit a wide temperature range of N_F phase, enantiotropic one in many cases. The general structure of investigated materials is shown below.



where:
$n = 0\text{-}5$
$m = 1\text{-}2$
$o = 0\text{-}2$
X_1 = O or CH_2
X_2 - X_5 = H, F, Cl or OMe

Figure 1: General structure of investigated materials.

Acknowledgements: This work was supported by the National Science Centre grant no. 2022/45/B/ST5/04093 and financed/co-financed by Military University of Technology under research project UGB 22-720.

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Viscous Mechano-Electric Phenomena in Ferroelectric Nematic Liquid

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Keywords: ferroelectric nematic liquid crystals, ferroelectric materials, mechano-electric response, mechano-electric liquid

Ferroelectric nematic liquid, which combines large spontaneous electric polarization with 3D fluidity, exhibits a range of mechano-electric[1] and converse mechano-electric phenomena[2–4]. We show that inducing the flow of the material confined to a glass container results in the reorientation of its electric polarization structure, as observed by examination of the second harmonic generation signal. This causes changes in the electrostatic configuration within the material leading to a direct mechano-electric response as observed in the 1-200 Hz frequency range via a simple demonstrator device. The ferroelectric liquid thus combines features that were previously only attributed to distinct materials, in particular, the mechanical compliance of a liquid and the well-pronounced mechano-electric transduction common for piezoelectric solids. A rich interplay of several distinct viscous mechano-electric phenomena results in a complex electric signal. Consequently, the results suggest a considerable applicative potential of the ferroelectric liquid spanning from sensitive tactile sensors to energy harvesting devices.

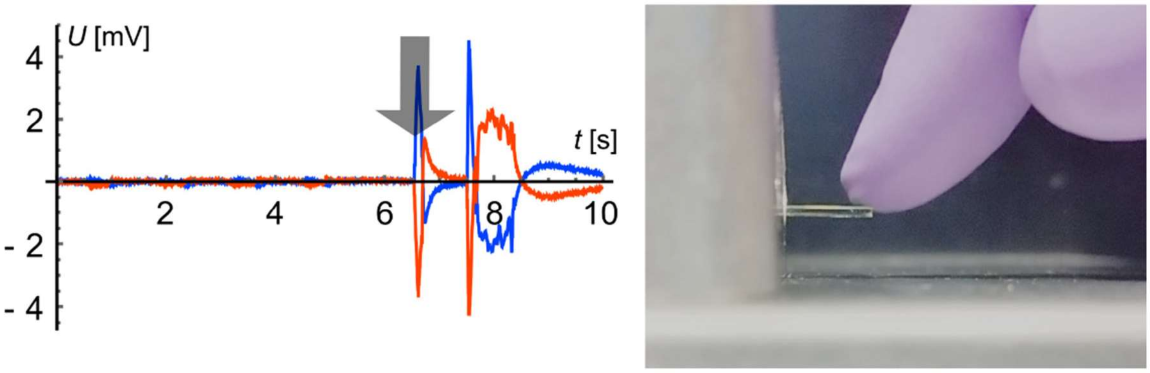

Figure 1: Electric signal obtained by deforming glass container filled with ferroelectric liquid crystal.

Acknowledgements: The study was funded from the European Union's Horizon 2020 research and innovation programme by the project MAGNELIQ under grant agreement no 899285 and by the Slovenian Research Agency (research core funding no. P1-0192).

The ferroelectric nematic liquid crystal material used in this work was supplied by Merck Electronics KGaA.

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C4

Dielectric, ferroelectric and flexoelectric properties

Deviations from Nematic Behaviour in Polar Nematic Liquid Crystals

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Keywords: Ferroelectric Nematic, Dielectric, Elastic Constant, Flexoelectricity

Since its experimental discovery in 2017, the ferroelectric nematic (N_F) liquid crystal phase has generated a large amount of interest in both fundamental and applied science [1,2]. The N_F phase has orientational order but lacks inversion symmetry and so exhibits bulk polarity. It is therefore important to consider how the effects of this molecular polarity manifest in the higher-temperature non-polar nematic phase (N), and whether the N bulk properties are affected.

We present temperature-dependance of the splay and bend elastic constants (K_{11}, K_{33}), real dielectric permittivity, and Freedericksz threshold voltage, V_{th}, in the nematic phase of a liquid crystal mixture (M5) that exhibits an enantiotropic N_F phase. Our results show an initial reduction in K_{11} and V_{th} as the temperature decreases, followed by a drastic increase in these values ~8°C above the intermediary nematic (N_X) phase. In contrast, K_{33} and dielectric anisotropy increase with decreasing temperature, similar to nematic materials 5CB and E7. At high temperatures close to $T_{N\text{-}Iso}$, good fitting to nematic models is displayed; however, the mixture shows strong deviations from this behaviour at lower temperatures on approaching transitions into the N_X and N_F phases. We attribute these deviations to contributions from flexoelectric coefficients which appear to become significant close to the N_F phase [3].

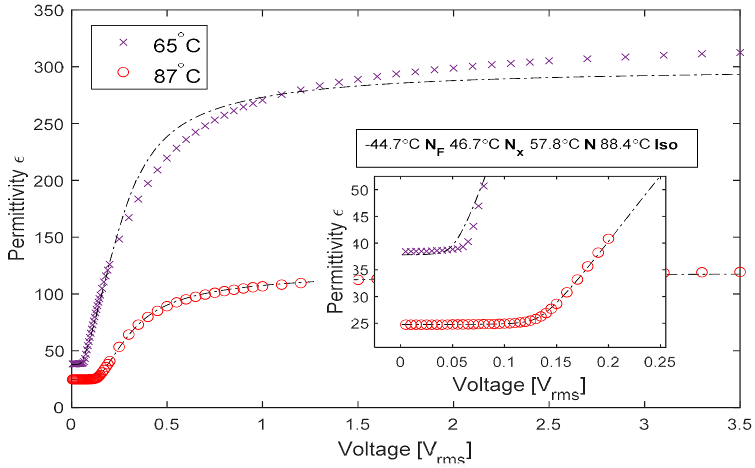

Figure 1: Graph of the real dielectric permittivity as a function of applied voltage in the nematic phase of M5, with nematic modelling showing deviations.

Acknowledgements: The authors would like to acknowledge the EPSRC and Merck for funding.

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Liquid piezoelectric materials: Linear electromechanical effect in fluid ferroelectric nematic liquid crystals

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Keywords: piezoelectricity, fluid ferroelectrics, ferroelectric nematic liquid crystals

The first demonstration of converse piezoelectricity in 3-dimensional fluids is presented by measuring a linear electromechanical effect in ferroelectric nematic liquid crystals. The observed piezoelectric coupling constant below $6\,kHz$ electric field is larger than $1\,\mathrm{nC/N}$, comparable to, or better than, values for the strongest solid piezoelectric materials.[1] Symmetry considerations indicate that the alignment of the ferroelectric nematic liquid crystal in our experimental study is not optimized, so the observed signal is arguably only a fraction of the theoretically achievable signal. Understanding the electromechanical response of ferroelectric nematics will enable mechanical energy harvesting and open up a new avenue for developing fluid actuators, micro positioners, and electrically tunable optical lenses.

Acknowledgements: This work was financially supported by US National Science Foundation grant DMR-2210083 and by the Hungarian National Research, Development, and Innovation Office under Grant NKFIH FK142643. The materials FNLC 1571 and FNLC 919 were provided by Merck Electronics KGaA, Darmstadt, Germany.

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Surface interface effects on the reorientation of smectic layers in surface stabilized ferroelectric liquid crystals

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We report the Smectic layer reorientation process in a surface – stabilized ferroelectric liquid crystal by surface interface and in combination with the measuring field. The process is investigated by dielectric spectroscopy and optical texture analysis in heating and cooling cycles under specified conditions in thin surface stabilized ferroelectric liquid crystal cells. The thickness of cell was maintained around 3.0 micrometre and homogenous alignment was obtained by polymer rubbed electrodes. The smectic layers are soft enough to be reoriented at the phase transition from the smectic phase to next higher temperature phase therefore the studies have been carried out near the chiral smectic C (SmC*) to chiral smectic A (SmA*) phase transition in heating and cooling cycles separately. We have found the different smectic layer molecular dynamics in heating and cooling cycles of material. It has been observed that in heating cycles, the surface effect phenomenon is dominant and in cooling cycles it is weak. The smectic layers can be reoriented to one side of the rubbing direction with one type of bias polarity and to the other by opposite polarity of bias field. The application of varying strength of AC field has revealed the existence of surface effect which in turn assist the reorientation of smectic layers on the application of DC bias at the same time. The study largely motivates the application of such FLCs in device of where the change in optic axis of the same device is required.

D

Novel Applications

D1

Functional materials for devices

Cholesterics: infinitely beautiful, mysterious, powerful

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Keywords: cholesterics, polymerization, multiple emulsions, selective reflection, mechanochromism, unclonability.

Despite being as old as liquid crystals themselves, cholesterics do not cease to inspire and challenge researchers, and their unique optical properties formed by tunable self-organization in combination with their fluidity offer powerful solutions to many of today's most pressing societal and technical problems. The opportunities to harness their extraordinary optics in innovative applications are rapidly expanding, not least thanks to three key related developments taking place over the last few decades: (1) the development of reactive mesogens that allow the self-assembled cholesteric structure to be transferred into a durable solid via polymerization; (2) the formulation of chemistries for easy fabrication of liquid crystal elastomers (LCEs), enabling the fabrication of mechanochromic cholesteric LCEs constituting a new paradigm in strain sensing; and (3) the advances in microfluidic multi-phase processing as well as 3D printing and fiber spinning, allowing cholesterics to be molded into form factors entirely different from the traditional flat panels of the display industry. In my talk I will describe how these tools allow us to leverage the chiral Bragg reflection of cholesterics to thwart counterfeiting and enable reliable and transparent supply chains [1], assist robots and Augmented Reality (AR) devices in understanding their environment [2], monitor tension in fibers in textiles and in knots [3], detect and monitor cracks in surfaces before they become dangerous [4], boost the sensitivity and versatility of rapid antigen tests [5], and even to make solar cells look great while keeping their performance almost intact [6]. I will draw from our own research in collaboration with internationally leading researchers in each of these fields to demonstrate that these are not just academic dreams but rather concrete plans that we are pushing hard to bring to the market.

Acknowledgements: I thank all current and previous members of the ESMP team for always pushing the envelope of our research field, as well as the European Research Council, the Fonds National de la Recherche Luxembourg and the Office of Naval Research Global for funding our research.

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Columnar LCs for delayed luminescence

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Keywords: columnar glass, room temperature phosphorescence, delayed fluorescence, triplet band gap, twisted pi electron system

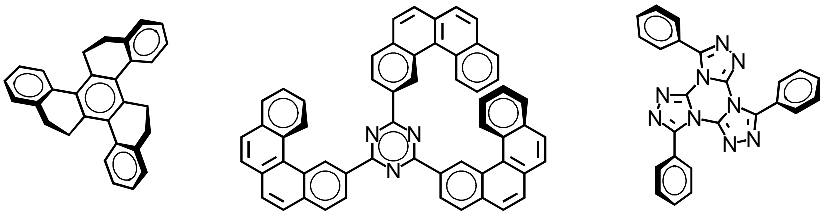
Roughly disk-shaped systems are common in chromophores that show delayed fluorescence (eg. TADF or TTA-DF) and organic phosphorescence, but considerable twist of the pi system is required as well to induce efficient HOMO-LUMO separation and thus first excited singlet and triplet states of similar energy.

Alignable but mechanically robust discotic liquid crystals such as hexagonal columnar glasses are of promise for anisotropic emission of delayed luminescence leading to enhanced light outcoupling out of diode devices. To induce a glassy LC state, a limited rotational flexibility of the disk-shaped aromatic core, including twisted configurations, is beneficial.

Liquid crystalline matrices for blue, white or full color emission that involves triplet states require aromatic pi systems with a very large T1-S0 gap to avoid quenching of a blue emitter's triplet states by the matrix.

Combining the partially contradicting geometric and electronic requirements to obtain delayed-luminescent columnar mesogens or glassy columnar matrices compatible with delayed-luminescent dopants is a challenge that requires careful optimization of twist and partial segmentation of the pi system.

Systems that have proven promising in our hands are substituted homotruxenes [1], triaryl-triazolotriazines [2] and triaryl-triazines [3]. An overview will be given over our current work with these systems.



The off-planar discotic cores homotruxene, tris(tetrahelicenyl)-triazine
and triphenyl-tristriazolotriazine

Acknowledgements: This work is funded by the Franco-Brazilian cooperation Capes-Cofecub 937-20 / Ph-C 962-20.

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Discovery of giant Cotton-Mouton effect in two-dimensional cobalt-doped titanium oxide liquid crystal and its application

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Keywords: 2D materials, Cotton-Mouton effect, Cobalt-doped titanium oxide, Light modulation, Interference color

Cotton-Mouton (CM) effect refers to a magneto-optical effect that can be used to pursue a non-invasive optical manipulation. However, the insensitive CM response requires a huge magnetic field, which is unacceptable in reality. The liquid crystals (LCs) with both high magnetic sensitivity and optical anisotropy, as promising CM media, are highly expected. Here, we discover a giant CM effect in two-dimensional cobalt-doped titanium oxide (2D CTO) LC. It possesses a record-high CM coefficient of 3.3×10^{3} $m^{-1}T^{-2}$ and transmitted interference colors. By varying the cobalt doping ratio and the geometrical characteristics, we propose that 2D CTO LC has a large optical anisotropy factor of up to 2.9×10^{-11} $C^{2}J^{-1}m^{-1}$ and a magnetic susceptibility anisotropy of 1.2×10^{-5} $m^{3}kg^{-1}$, which collectively contribute to its sensitive response. Furthermore, various optical components based on 2D CTO LC are demonstrated, such as waveplate, optical attenuator, stress indicator, and DUV modulator. This work paves the way for the practical application of LC-based CM effect devices.

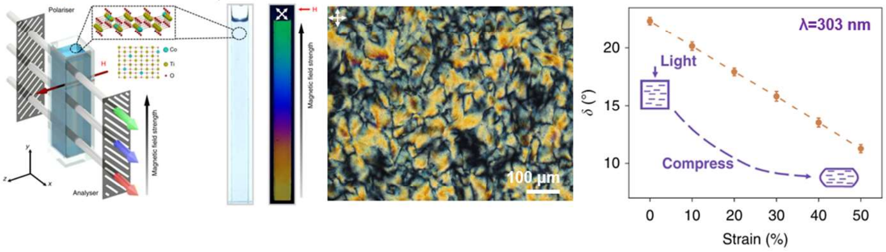

Figure 1: 2D CTO LC and its optical components

Acknowledgements: This work is supported by the National Natural Science Foundation of China (Nos. 51920105002, 52125309, 52273311, 51991343, 51991340, and 52188101), Guangdong Innovative and Entrepreneurial Research Team Program (No. 2017ZT07C341), National Key R&D Program (No. 2018YFA0307200), National Program on Key Basic Research Project of China (No. 2020JCJQ-ZD-06312), Shenzhen Basic Research Project (No. JCYJ20190809180605522, JCYJ20220818100806014, WDZC20200819095319002, WDZC20231128154552002), ‘2017 Graphene Manufacturing Innovation Center Project’ (No. 201901171523), and Shenzhen Pengrui Young Faculty Program (No. SZPR2023002).

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Dynamics of nanorod assemblies in liquid crystal topological defects

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Keywords: liquid crystals, nanoparticles, self-assembled, diffusion, instability

Smectic liquid crystals (LCs) host a variety of topological defects(TDs) [1] where nanoparticles can be confined and organized [2]. We have shown that the confinement induced by smectic patterns made of oriented ribbon-like grain boundaries (2D topological defects) leads to the formation of oriented ribbons of fluorescent nanorods (NRs) [3]. We now evidence a peculiar dynamics of these assemblies of NRs within the smectic TDs. It has been shown in the past that in LCs matrices, the dynamics of particles often departs from a Brownian-like diffusion [4]. Our study addresses the issue of soft confinement induced dynamics within smectic TDs. It is interesting because firstly structural information on the smectic topological defect matrix may be indirectly obtained. Secondly, an active modification of the NR assembly structure may become triggered by their dynamics. We combine optical and fluorescence microscopy and synchrotron-based grazing incidence X-ray scattering (GISAXS) to study the structure and dynamics of the NR assemblies. A unidirectional dynamics is revealed for the ribbons along the defects in relation with a strict confinement of the NRs within the defects. It is characterized by two kinds of motion: small scale fluctuations (up to100nm) and jumps between two equilibrium positions (150nm to 350nm). This behavior is reminiscent of the sub-diffusive dynamics obtained with particles confined in polymer networks whose mesh size is of the order of the particle diameter [5], showing that the subdiffusive motion of the NR assemblies in the smectic defects is traplike. It is observed that the NR assembly size and density determines the fluctuation and jump values, confirming that the smectic elasticity induced by the presence of the NRs, whose size is larger than the defect core drives both fluctuation and jump values. This allows us to extract the exact smectic distortion induced by the confinement of each NR assembly in the defects [6] together with the spatial variation of these distortion. We demonstrate that to avoid this confinement drsubdiffusive dynamics, the temperature has to be increased close to the smectic/nematic phase transition. A continuous diffusive motion of the NR ribbons is thus induced, in relation with the increase of the defect core size. Connection between neighbouring ribbons becomes possible to finally elongate the ribbons up to lengths reaching easily 10 micrometers. This may allow in the future to connect two electrodes by single ribbons for future studies of transport properties within nanoparticle ribbons.

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Enhancing Solar Cell Aesthetics with Cholesteric Liquid Crystals: Arbitrary Coloring of Photovoltaic Panels with Maintained Efficiency

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Keywords: Photovoltaics, structural color, liquid crystals, aesthetics, conversion efficiency

Excessive burning of fossil fuels has dangerously raised the earth's temperature causing untold environmental damage, making a switch to renewable energy technologies vital. Over a third of the final energy consumption is assignable to buildings, which is why the EU aims for all new buildings to be net-zero-emission.[1] Solar photovoltaics (PV) panels are ideal sustainable energy building elements, for electricity generation and/or for heating, but their visible impact is currently prohibitive for many installation options, e.g., on the façades of buildings. The inherent monotone blue/black colors of standard PV panels are a devastating blow to architectural aesthetics, rendering building-integrated panels (BIPV) challenging.[2] To realize the full potential of BIPV, panels must be made visually pleasing and be available with any pattern or color, yet without compromising power conversion efficiency (PCE). The latter criterion means the coloring must have minimum impact on incident light transmission to the PV panel's solar cells. Our research reveals that a properly designed coating of cholesteric liquid crystal (CLC) transforms black solar panels into surfaces of customizable color with minimum impact on efficiency. The self-organized helical modulation of CLCs produces structural color without absorption or indiscriminate scattering, minimizing light loss. All light outside the reflection band is fully transmitted and even in the reflection band 50% is transmitted due to the CLC selection of only one circular polarization, unlike the interference filters used in today's commercial-colored modules. Most conspicuously, we demonstrate the generation of non-spectral colors by combining red (R), green (G), and blue (B) pixels through additive RGB color mixing, as shown in Figure 1. Normally non-spectral coloring requires the use of absorptive and scattering pigments, resulting in a huge reduction in PCE. We argue that the principle can be developed to make solar panels with arbitrary full-color images, allowing them to be aesthetically integrated into building façades as well as roofs in a way that is fully acceptable by the public, with retained efficiency of operation. Thereby, cholesteric liquid crystal can be the enabling key to reach the full potential of BIPV.

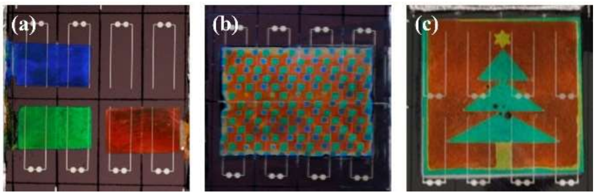

Figure 1: Macroscopic photograph of (a) R, G, B retroreflection colored, (b) red-green-blue-pixelated, (c) Christmas tree patterned solar cell.

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From slow to speedy: laser-driven robots swim faster with algorithms guidance

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Keywords: liquid crystal elastomer, optimization, smart material, soft robot

LCEs are materials that combine the properties of liquid crystals and elastomers (elastic polymers). Similar to liquid crystals, they can reversibly change molecular alignment under external stimuli, but in LCEs, this induces macroscopic deformation, making them ideal components for soft robots. We present centimeter-scale laser-driven swimming robots inspired by our previous work - caterpillar-like crawling ones [1]. Their 'bodies' are made of LCE, which deforms into an accordion-like shape when heated. By scanning the LCE with a laser, we can heat only a small area at a time and induce a traveling wave that propels them (see Fig. 1).

During experiments, we aimed to answer the question: How can we make our robots swim faster? There are several parameters we can adjust, including laser power, robot size, concentration of dye absorbing the laser light, and more. We employed two bioinspired algorithms, genetic algorithm and particle swarm optimization, to obtain faster robots. For each approach, we conducted separate experiments starting with the randomization of parameters for the initial population of robots and measured the speed of each robot. We then repeated the following steps: generating the next population using the algorithm based on previous velocities and measuring the velocity of each individual in the new population (see Fig. 1). By following this procedure, we improved the speeds from 1.7 to over 10 cm/min. We will present the parameters of the algorithms used, the observed modes of locomotion (e.g., self-oscillation of the robot), and compare the results obtained with both algorithms.

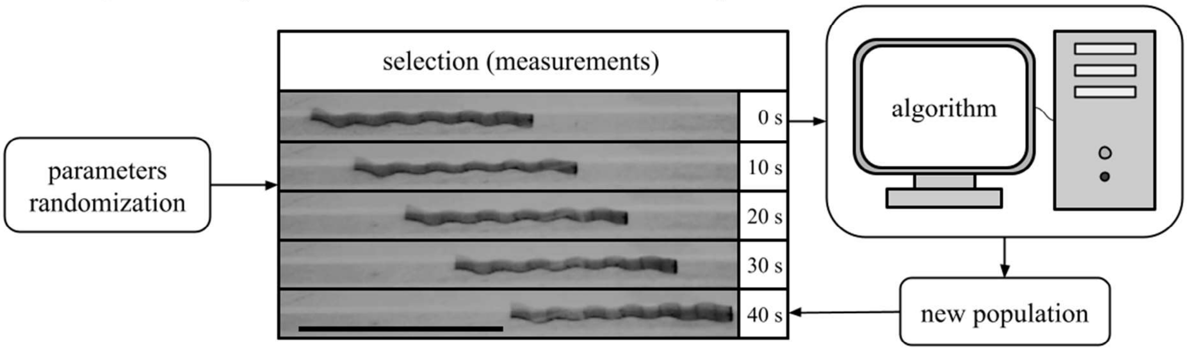

Figure 1: Optimization scheme. The 'selection' rectangle shows frames from the recorded swimming motion of single robot (scalebar: 1 cm).

Acknowledgements: This work was supported by the Polish Ministry of Science and Higher Education (MNiSW) with grant “Diamentowy Grant” No. DI2016 015046.

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High electrical conductivity in an insightfully engineered luminescent columnar liquid crystal for solution-processable nanoelectronics

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Keywords: discotic liquid crystals, self-assembly, solvatochromism, organic semiconductors, hole-transport

Recent advancements in the field of organic semiconductors emphasize a challenge of achieving the perfect balance between effective charge-carrier transport and solution-processability. In this context, discotic liquid crystals (DLCs) are a class of self-assembling materials harmonizing supramolecular order and dynamics in a system that can potentially address the challenge.[1] In this work, we envision a minimalistic design strategy for a cyanovinylene-integrated pyrene-based DLC (**PY**) to exhibit a room-temperature columnar hexagonal mesophase and a narrow band gap for efficient semiconducting behavior. Even at low values of applied voltage, **PY** exhibited superior charge extraction ability from the contact electrodes, achieving an electrical conductivity of 3.22×10^{-4} S/m, the highest reported value for any undoped DLC film in a vertical charge transport device. Its hole mobility values were comparable to the best organic hole transport layers (10^{-3} cm^2/Vs). In analogy with device performances, photophysical studies were correlated with carrier transport in the excited state induced by charge injection, substantially corroborated by theoretical studies on the molecular geometry, frontier orbitals and reorganization energies.

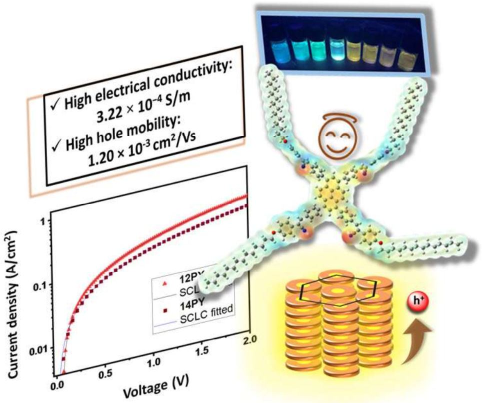

Figure 1: Representation of the charge transport and luminescence in the columnar DLC **PY**

Acknowledgements: Project CRG/2019/000901/OC is acknowledged for funding. The presenting author acknowledges IISER Mohali for her fellowship and departmental/central research facilities.

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Interactive liquid crystal polymers for soft robotics and haptics

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Keywords: haptics, interactive materials, liquid crystal polymers, liquid secretion, dynamic surface topographies

We propose the utilization of a liquid crystal polymer network (LCN) for soft robotic fucntions, where diverse molecular components are arranged within a two-dimensional coating. Notably, the LCN surface exhibits dynamic deformations into predefined topographic patterns triggered by factors such as temperature, light, and electric fields (1). These microscopic alterations have a significant impact on macroscopic aspects like tribology, haptics, laminar fluid mixing in microchannels, and guided cell growth. Additionally, our LCN coating incorporates a robotic-relevant function, allowing controlled liquid secretion under UV irradiation or through an AC field (2). This controlled release capability opens avenues for applications such as lubrication, regulated adhesion, drug delivery, and agricultural, antifouling in marine and biomedical devices, as well as personal care and cosmetics. This comprehensive toolbox forms the basis for designing two-dimensional soft robots tailored for environments where human-machine interactions occur.

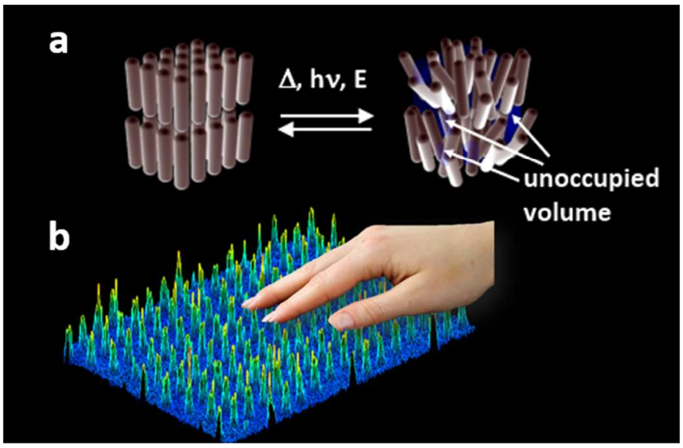

Figure 1: Liquid crystal polymer networks used for haptics. (a) principle of the anisotropic deformation of liquid crystal polymer. (b) surface structures generate touch feedback.

Acknowledgements: The author acknowledges the discussion with Professor Dirk J. Broer

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New Bent-Core Liquid Crystals Applicable in Gas Sensors

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Keywords: Liquid Crystals, Sensors, Electrochemistry, Organic Synthesis

Liquid crystals (LCs) opened an exciting new research area seeking applications beyond the display technology, alike nonlinear optics, photonics, and drug delivery systems, among others. The innate fragility of mesophases and their inherent sensitivity to various external stimuli offer intriguing sensor applications.[1] Thus far, heterojunction sensors have been fabricated by depositing sequentially a molecular semiconductor and lutetium bis-phthalocyanine thin film in a bilayer configuration on ITO interdigitated electrodes (IDE).[2] The organic heterojunction effect, causing accumulation of mobile charge carriers at the organic-organic interface, results in the enhancement of interfacial conductivity that can be exploited to fasten the charge transfer during gas-sensing material interaction.[3]

In this study, we deal with the synthesis of new bent-shaped LCs based on the previously established central unit,[4,5] and present a subsequent study on their application in electronic organic devices based on ITO IDE (Figure 1). The materials were fully characterized, including X-ray analysis, DSC and POM studies. Subsequently, our aim is to investigate new heterostructures consisting of a bilayer assembly of LCs and $LuPc_2$ for ammonia sensor development. Ammonia sensing has been studied giving response curves at successive exposures with NH_3 concentration in the range of 10-90 ppm for six sensors. Generally, the new LC-based devices demonstrate significant advantages over the established technologies, solution processability and simple drop casting technique for thin layer deposition.

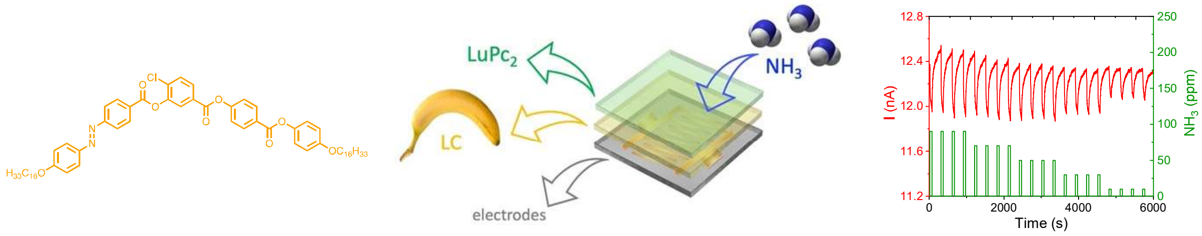

Figure 1: Schematic view of a molecular bilayer heterojunction on ITO IDE.

Acknowledgements: This work was supported by the French Ambassy through the Cotutelle fellowship program (Barbora Jansová) and Czech Science Foundation (reg. No. 22-16499S).

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Polymerization of twist-bend nematic textures for electro-optical applications

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Keywords: twist-bend nematic; polymerization; optical gratings; smart glass

The twist-bend nematic (N_{TB}) phase, discovered in 2011 [1], has since been the subject of many studies to understand its structure, elastic properties, and response to electric fields [2], and has been reported with many compounds [3]. However, despite its promising physical properties, this phase has not found applications yet because it is often metastable and usually crystallizes at room temperature [4]. Due to its heliconical structure, the N_{TB} phase is fairly similar to the smectic A (SmA) phase since both are layered phases with comparable periods. Consequently, some defects commonly observed in the SmA phase, such as focal conic domains, are also observed in the N_{TB} phase. Furthermore, like the SmA phase, the N_{TB} phase cannot be reversibly aligned with an electric field. Therefore, to tackle this issue, we applied an approach previously used with SmA liquid crystals [5] which consists in polymerizing the defects of the N_{TB} phase to maintain them in the nematic (N) phase. We thus extended the analogy between SmA and N_{TB} phases and stabilized various N_{TB} defects (focal conics, ropes, double helices) in the N phase. This process allows exploiting the N_{TB} phase for promising electro-optical applications such as optical gratings and privacy control using smart windows (Figure 1).

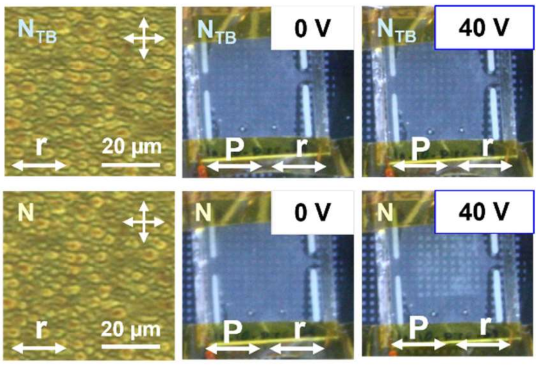

Figure 1: Focal conic domains polymerized in the N_{TB} phase (top row), heated to the N phase (bottom row) and submitted to electric fields. Privacy control is thus achieved in the N phase.

Acknowledgements: The authors thank Frédéric Mondiot for helpful discussions.

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SHG-active chiral bipyrimidine-based liquid crystalline thin films for 3D data storage

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Keywords: Bipyrimidine, Liquid crystal, Chirality, Thin films, Nonlinear optic, Data storage

The use of organic chromophore thin films in nonlinear optics is growing due to their ease of processing, versatility and tunability, and offers increasing potential in optical communication, optical switching, frequency conversion and more. In particular, SHG organic thin films have attracted considerable interest for data storage due to their potential for high-density information coding.[1] With this in mind, we have developed a strategy for functionalizing 3D organic octupoles with chiral chains to generate non-centrosymmetric liquid crystalline thin films that enable the development of highly active SHG materials without the need for corona polishing or tedious deposition techniques (Figure 1, left).[2-4] Recent developments have highlighted the possibility of efficiently recording data on these SHG-active liquid crystalline thin films by three-photon absorption, paving the way for 3D optical data storage (figure 1, right).

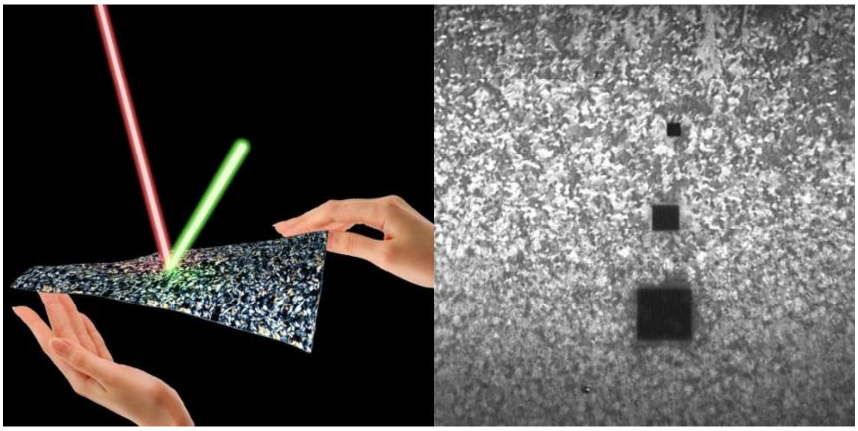

Figure 1: Illustration of the SHG signal emerging from an LC thin film (left), Data recording in an SHG-active liquid crystalline thin film (right).

Acknowledgements: ANR (3D-ODS), Région Bretagne (3D-STORE)

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Spontaneous emergence of structural patterns in chiral bent-core liquid crystal

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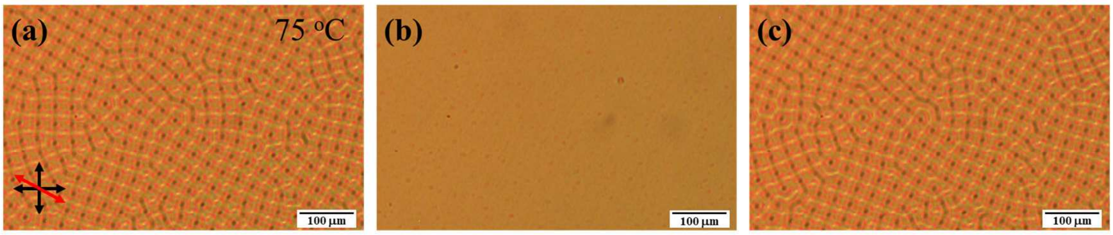
Keywords: Bent-core liquid crystal, Helix undulation, Spontaneous pattern, Wedge cell

The self-assembled architecture of liquid crystals (LCs) manifests a distinct variety of functional microstructural patterns which make them invaluable in advancing photonic and electro-optic devices [1]. Similar to the electroconvection pattern, the helix undulation technique generates uniform periodic structural patterns in cholesteric LCs (CLCs). However, for practical application, there is a requirement for stabilization of such periodic patterns. The stabilization of periodic patterns by electrode decoration, polymerization and using hybrid alignment layers reduces the tunability and working efficiency [2]. In order to meet the specifications for developing high-end photonic devices, a suitable LC material is required to induce spontaneous periodic patterns with a broad range of tunability. In this work, we investigated a chiral system consisting of a bent-core LC compound, having moderate polar order and possessing a frequency and temperature-dependent crossover nature in dielectric anisotropy. The field-induced development of 1D, and 2D patterns and their spontaneous appearance at higher thicknesses are investigated in both uniform and wedge-shaped cells. The formation of undulation patterns is explained based on the confinement ratio and influence of the alignment layer. In addition to a moderate ferroelectric polar order in the bulk of the LC system, larger contribution of effective elastic energy plays a crucial role in spontaneous undulation patterns [3]. Fig. 1 demonstrates that applying an electric field with high frequency immediately resolves the pattern and after the complete removal, the pattern gradually return after certain time period. This may be attributed to the influence of frequency-dependent dielectric anisotropy. The understanding of the appearance of both the field-induced and spontaneous patterns and the tunability offers a facile approach for designing potential devices in controlled adaptive optics.



Without EF   20 V, 10 kHz   After removal EF

Figure 1: Optical textures for the prepared CLC mixture filled in wedge cell, (a) spontaneous pattern at 75 °C, (b) after and (c) removal of EF of 20 V, 10 kHz.

Acknowledgements: The authors thank Defence Research and Development Organization, India for funding the project vide grant DFTM/03/3203/P/01/JATC-P2QP-01.

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Towards Glassy Columnar LC Matrices for Anisotropic TADF

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Keywords: Triphenyl-triazine, Columnar Glass, Anisotropic emission, Delayed fluorescence, Triplet band gap

Alignable anisotropic columnar and nematic liquid crystals made of disk-shaped molecules have great potential for light emitting devices, because by aligning the emitter dipoles with respect to the device surfaces,[1,2] the losses due to inefficient light outcoupling may be significantly reduced.[3] To maintain the homogeneously aligned configuration in a robust solid, the liquid crystalline order can be frozen through a glass transition above ambient temperature. Furthermore, to function as a matrix for TADF emitter materials that rely on reverse intersystem crossing between excited triplet and singlet states, the matrix material should exhibit a triplet excited state energy that is larger than that of the emitting guest molecules. Ideally, the T1 state energy should be around or above 3 eV to allow emission at all visible wavelengths including blue. Triphenyl-triazine has previously been identified as suitable large-T1-energy core with threefold symmetry to allow the elaboration of liquid crystalline derivatives, and carboxylic alkyl ester groups have proven to be appropriate substituents to induce high viscosity[4] (Figure 1). In triaryl-triazines, the rotational flexibility of the three singly-bonded aryl substituents is prone to hinder crystallization and favor the formation of a glassy state. Whilst phenyl substituents proved too small to induce a glassy state above room temperature, large aryl groups such as [4]helicenyl led to a considerably shortened T1-S0 energy gap.[5] Naphthyl thus appears as a convenient aryl moiety, and therefore we have elaborated various trinaphthyltriazine tri- and hexaesters to combine adjusted phase behavior with good optoelectronic characteristics.

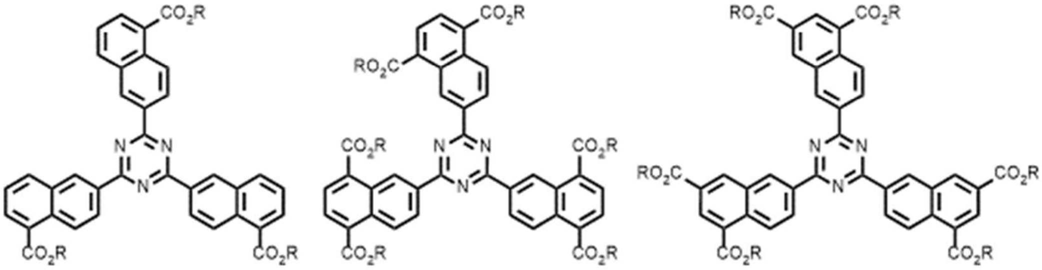

Figure 1: Configurationally flexible columnar trinaphthyl-triazines; R = short alkyl.

Acknowledgements: This work is funded by the Franco-Brazilian cooperation Capes-Cofecub 937-20 / Ph-C 962-20, and by CNPq.

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Tunable Functional Liquid Crystal Optical Elements

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Keywords: active optics, adaptive lens, variable attenuator, smart windows, tunable color generation, plasmonic metasurface

Active optical elements such as adaptive lenses, variable attenuators, and tunable color filters based on liquid crystals are emerging technologies in optics and photonics. They add more powerful functions to the optical systems, and have wide applications in imaging, vision care, smart windows, AR/VR displays, etc. In this talk, we are going to report some of our recent progress in these active optical elements.

We have developed broadband (400-700nm), polarization independent, high-performance tunable attenuators with low operation voltage (<24 volts), high contrast ratio (>200), and fast response (~ subsecond) by using a liquid crystal mixture made up of nematic liquid crystal, chiral dopant, and dichroic dye.

We will present a scheme for tunable structural color generation by using a liquid crystal-filled plasmonic metasurface. The tunability is due to the combination of the polarization angle rotation effect of the twisted-nematic liquid crystals and the refractive index modulation through the reorientation of the liquid crystals near the metasurface. A record color gamut of 60.7% standard RGB region, equivalent to 43% NTSC area has been achieved in the design in reflection mode by tuning the bias voltage. The color gamut is nearly 4 times wider than the previously reported result.

Acknowledgements: The author thanks the support from Fudan University through the Research Initiation Project (IDH2323007Y) and the support from Shanghai Frontier Base of Intelligent Optoelectronics and Perception.

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D2

Displays, devices, optics and photonics

Active planar chiro-optic devices with ultra-broadband tunability and invertible chirality

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Keywords: geometrical phase, cholesteric liquid crystal, orbital angular momenta, photonic bandgap, helix inversion, molecular motors

ABSTRACT: Active planar optical elements exhibiting compactness and miniaturization are highly sought after in replacing of traditional bulky and static devices. Specifically, chiro-optic-based geometrical phase elements (GPEs) have garnered extensive attention due to their versatile beam shaping functionalities, including amplitude, wavelength, polarization, and angular momentum. In this study, we employed micropatterned photoalignment technique to fabricate various GPEs utilizing light-stimulatable-molecular-motor-based cholesteric liquid crystal (CLC) doped with. When the incident light's wavelength falls within the CLC's photonic bandgap, the reflected light undergoes phase modulation determined by the distribution of micro-patterned CLC directors on the substrates. Through external light stimulation, the concentration of two distinct isomers of molecular motors with opposite chirality undergoes changes, enabling continuous and reversible tuning of the working band and chirality of CLC (Some results are shown in Figure 1.). This work offers future guidelines for achieving complete dimensional control of light in self-organized soft materials.

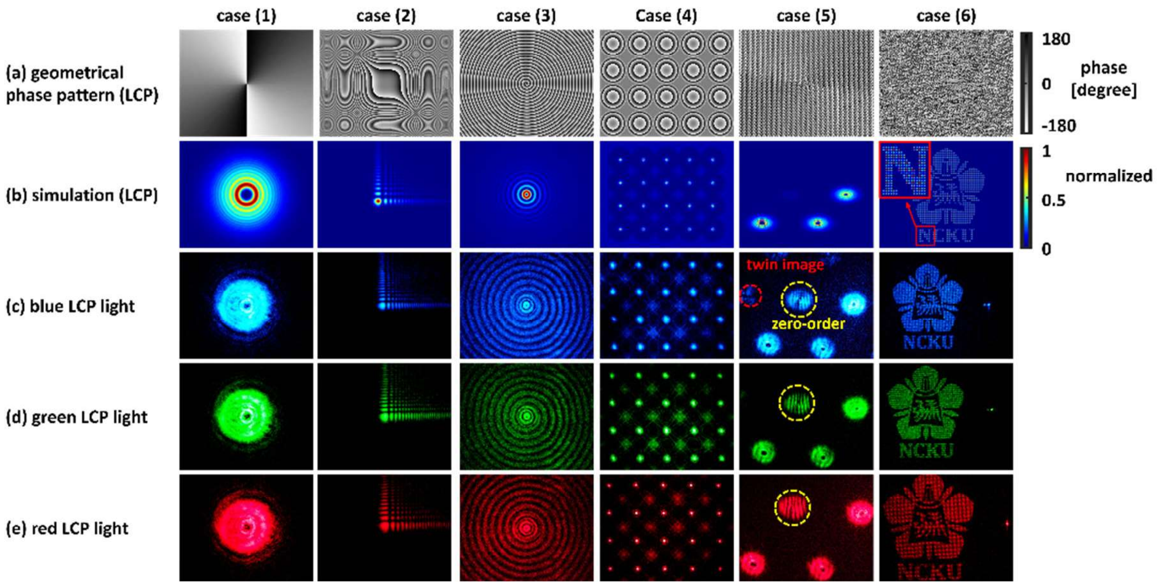

Figure 1: Demonstrations of five different GPEs based on five different geometrical phase patterns (a), where case (1) is a vortex phase with a topological charge modulus of 2, case (2) is an Airy phase, case (3) is a Bessel-vortex phase with a topological charge modulus of 1, case (4) is a micro lens array phase with a focal length 35 cm, case (5) is a vortex array phase grating with charge moduli of 1, 2, and 3, and case (6) is a computer-generated hologram. Simulated (b) and experimental far-field diffraction patterns of reflected LCP light at wavelengths of 488 nm (c), 532 nm (d), and 633 nm (e).

ACKNOWLEDGEMENTS: The authors would like to thank the National Science and Technology Council (NSTC) of Taiwan for financially supporting this research under Grant No. NSTC 112-2112-M-006-021 & NSTC 112-2221-E-006 -168 -MY3.

Additive Manufacturing of Liquid Crystal Photonics Technologies

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Keywords: 3d printing, two-photon polymerization, inkjet printing, liquid crystal optics

Additive manufacturing methodologies such as 3D printing and drop-on-demand techniques enable new functionality and behavior to be unlocked in traditional liquid crystal (LC) device architectures. In this presentation, I will present our work on two photon polymerization direct laser writing (Figure 1) and drop-on-demand printing to demonstrate how these methods can be used to fabricate new optical components from LC resins. For the direct laser writing, I will show how this technique can be used to write polymer networks of different shapes and sizes into LC devices to create a broad array of different optical elements including diffraction gratings, computer generated holograms, and optical aberration correctors [1 - 6]. Alongside demonstrations of devices enabled through the use of laser writing, I will also present some of our work on novel LC optical elements that have been fabricated using drop-on-demand printing functioning in either an inkjet or electro-hydrodynamic mode. Results will be presented that showcase how these printing techniques can be used to fabricate optical vortex beam generators, Skyrmion beam generators and more. To conclude, I will consider how these techniques could be combined in the future to form new device technologies.

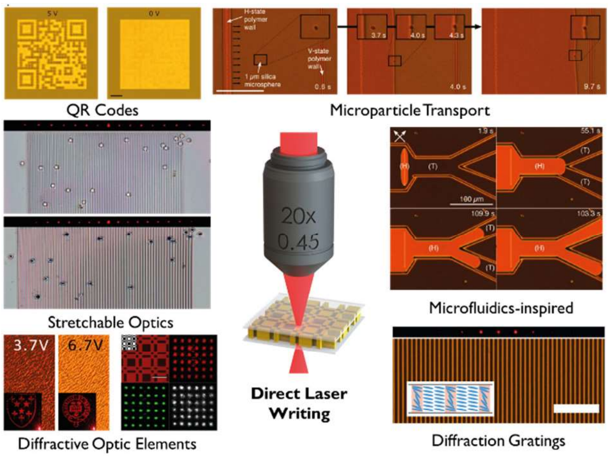

Figure 1: Laser writing in liquid crystal devices.

Acknowledgements: This work has been supported by Grant EP/R511742/1, The John Fell Fund (Oxford University Press), The Royal Society (U.K.), and Merck (UK).

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Alignment of Columnar Liquid Crystals: A Novel Approach for Enhancing Organic Solar Cells

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Keywords: Columnar Liquid Crystals, Organic Solar Cells, Homeotropic Alignment.

Organic solar cells (OSCs) are an interesting option to reduce environmental impact. Their primary advantage lies in the creation of portable and flexible devices that are lightweight and cost-effective, making their use accessible in everyday life. Despite the progress made in solar cell technology, there remains a lack of understanding regarding the influence of molecular alignment in these structures. One class of material that can be aligned to application in OSCs are the thermotropic columnar liquid crystals (ColLCs), especially those with perylene diimide (PDI) centers. These materials exhibit mesomorphic properties that vary with temperature, allowing molecular alignment. When confined between surfaces and subjected to temperatures nearing the isotropic phase, ColLC molecules become more fluid, enabling them to self-organize in a face-on orientation. This leads to an enhancement in their charge transport efficiency [1], [2]. Here, we have studied the influence of the alignment of a room temperature ColLC based on benzo-PDI center to act as the acceptor material in a blend with PFO-DBT polymer as the donor. Aligned samples exhibited higher absorbance and photoluminescence (PL) intensity compared to nonaligned samples. In both cases, aligned and nonaligned films, a significant reduction in ColLC emission was observed with increasing proportion of polymer in the mixture. Moreover, various concentrations of the solvent additive 1-8 diiodoctane (DIO) were incorporated into the mixtures, resulting in an observed increase in film crystallinity as DIO concentration was increased. As another part of the work, the molecular alignment of the ColLC was investigated in the structure of a solar cell as cathode interlayer (CIL). In this case, the ColLC was fully aligned in a face-on orientation on the top of a donor:acceptor photoactive layer consisting of the P3HT:ICBA blend. This study marks the first-ever report of a fully face-on aligned CIL in organic solar cells. The alignment of the ColLC resulted in a significant enhancement in power conversion efficiency (PCE) compared to non-aligned CIL. Furthermore, the PCE of the device with the aligned CIL exceeded that of the device without any CIL.

Acknowledgements: CAPES, CAPES-COFECUB Project, CNPq, and INCT/INEO.

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A Unification of the Four LCD-Modes such as the ECB, VA, IPS, and FFS-LCDs in their Electro-Optical Effects Accompanying Extra Geometrical Phase Advancement and Temporal Effect by Adopting Asymmetric Optical Compensation

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Keywords: Unification of four LCD operations, ECB, VA, IPS, and FFS-LCDs, Asymmetric optical compensation

1.Introduction: In a previous paper, we investigated the generation of extra geometrical phase advancement accompanying a rapid response speed in the switching off process in the asymmetric optical compensation in the IPS and the FFS-LCDs. [1,2] In this presentation, we update by including the ECB and the VA LCDs and we report a unified treatment of those four LCD-Modes in their optical transmissions and asymmetric optical compensation effects. Until now, these LCDs are treated as the different types.

2.Common shapes in the equations of optical transmission and V-T curves for these LCDs
In the normally white mode LCDs such as the ECB and the IPS -LCDs, the equations for the optical transmissions for the single cell reds $T_1=\sin^2(x)$, where x is the variable; in the ECB-LCD x is the polar angle θ_1 or phase angle δ_1, where as in the IPS-LCD x= ϕ_1.
In the normally black mode VA-LCD the $T_1=\cos^2(x)$, where x= θ_1, or δ_1.
The variables can be replaced with the operating voltages. that gives V=T curves.

3.Common shapes in the equations of optical transmission and V-T curves for these asymmetric LCDs optically compensated LCDs. In the IPS-LCD, the, switching angle is ϕ_1 and the setting angle of the compensator will be:$\phi_2=3\pi/4-\alpha$, then $T_2=\cos2\{2(\phi_1+\alpha)\}$, with this system and by taking as α= 6 degrees, we got twofold response speed over the single cell. When a=0, then the system is symmetric, thus we have no temporal effect. [1,2]
In the ECB, when we chose the phase angle of the compensator as $\delta_2=\pi/2+\alpha$,
then we got a slow response in the switching off process. For this reason, we chose $\delta_2=\pi/2-\alpha$ for getting twofold high -speed response. [1,2]

4.Common features in plain switching. As well known in the IPS-LCD, the switching is made in the x-y plain, while in the VA and ECB LCDs the switching is done in the x'-Z plain, where the x' axis directed with an azimuthal angle of $\pi/4$.These common features results in in the common shapes of T_1 and T_2.

5.We have developed a computer-controlled dynamic compensator using an LC-cell as an A-plate; this device enables controlling α at any desired instantaneous time. [1,2]-

6.Common simulation- results in comparison of the switching behaviors

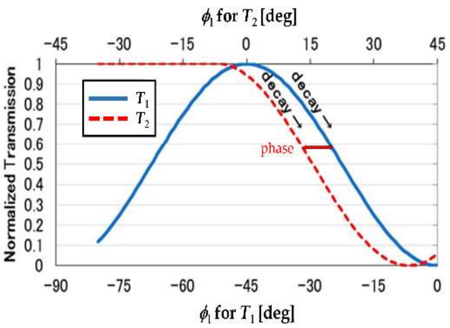

Figure 1shown on the left part is a simulation result that making a comparison between 1-T_1 and T_2, where the latter has an advanced phase α=6 degrees in the switching angle in the switching off process, where it is recognized a finite gradient in the beginning (at the top-center), whereas the curve for the single cell has no derivative; this gives the understanding of the rapid response speed of the asymmetric optical compensated LCD.

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Background- and Angle-Independent Intense Structural Color from Black Dye Infusion of Cholesteric Spherical Reflectors

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Keywords: cholesteric liquid crystal, dye absorption, pigments, camouflage

Many species in nature exhibit fascinating colors known as structural color, which arise from the interaction of visible light with periodic nanostructures and the ability of melanin to absorb light [1]. This remarkable color-creation mechanism of nature has been an inspiration for the design of artificial structural color materials [2]. The major drawbacks of most efforts to date are that the observing colors change depending on the viewing angle and the light scattering kills/ significantly reduces the color intensity. That is why bright structural colors are usually achieved on black backgrounds and immersed in the index-matching binder [3,4]. Thus, it remains a challenge to develop an effective method to produce bright structural colors independent of background and viewing angle.

In this work, by shaping a cholesteric liquid crystal into shells, polymerizing it into glassy solid, and then infusing the shells with black dye, we are able to overcome the previous challenges. Even in the absence of an index matching environment, the dye-infused Cholesteric Spherical Reflectors (d-CSRs) produce discrete pixels of intense, saturated color because the spherical shell geometry effectively eliminates the viewing angle dependency, provides omnidirectional retroreflectivity, and the black dye absorbs all randomly scattered light. Moreover, non-spectral colors can be produced by mixing d-CSRs with different retroreflective colors. In addition to successfully controlling dye infusion, we demonstrate our efforts for preparing arbitrary patterns, camouflaging them in a similar colored background, and revealing the hidden information by using the circular polarization selectivity of CSRs with a basic optical read-out design.

Acknowledgements: This work was funded by the Institute for Advanced Studies (IAS) of the University of Luxembourg.

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Chiral-nematic cells with conical anchoring for wide-range adjustment of light polarization parameters

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Keywords: chiral nematic, conical anchoring, light polarization, photosensitive chiral dopant

Chiral-nematic liquid crystals (CLCs) are of wide application in the optical and photonic devices due to their unique physical properties provided by the helicoidal orientational structure of director. This allows using CLCs to control the polarization of transmitted light. However, the complete control of light polarization in the typical LC devices is not possible because of the strong tangential or homeotropic anchoring of LC to the substrates.

In the present paper, the continuous tuning of the orientation of photosensitive LC under hybrid tangential-conical surface anchoring has been demonstrated owing to the control radiation and electric field [1]. CLC cells based on the nematic mixture LN-396 doped with the left-handed chiral dopant S5011 and the right-handed composite photosensitive chiral dopant cChD [2] have been studied. The strong tangential anchoring on one substrate and the conical boundary conditions on another one [3] allow for smoothly changing the twist angle φ_{dir} of CLC structure. The director twist angle and, consequently, the polarization azimuth ψ of the probe beam passing through the CLC cell was operated by the balance of ultraviolet (365 nm) and blue (430 nm) radiation. The ellipticity ξ of light polarization was controlled by the applied voltage. When the linear polarization of light is perpendicular to the director at the input of LC cell (Figure 1, *Scheme 1*), the system can operate as a photo-controlled achromatic rotator (Mauguin regime) of light polarization over the entire visible range. If the polarization of the incident probing light is oriented at an angle of -45° to the director at the input of LC cell (Figure 1, *Scheme 2*), then it is possible to smoothly adjust the polarization parameters of transmitted light ψ in the range [-90°; +90°] and ξ in the range [-45°; +45°].

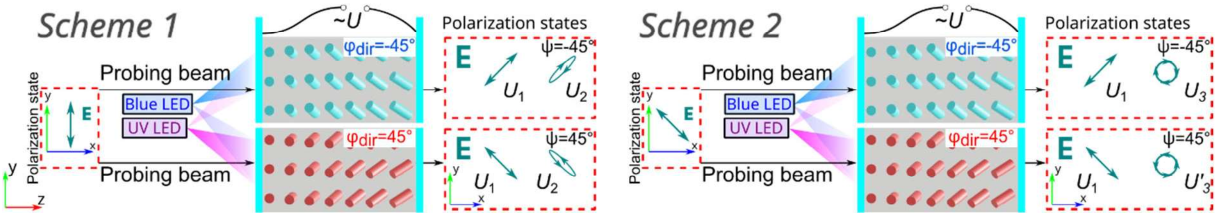

Figure 1: Schemes to control polarization of light transmitted through the CLC layer

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Development of highly sensitive photorefractive liquid crystals and their application to laser ultrasonics

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Keywords: Photorefractive effect, flexoelectric liquid crystals, ferroelectric liquid crystals, laser ultrasonics

Laser ultrasonics is a measurement technique that uses laser pulse irradiation to generate ultrasonic vibrations, which are then detected by another laser. Widely employed ultrasonic techniques use piezoelectric devices to generate and detect ultrasonic vibrations. Although these devices are highly sensitive, they require direct contact between the piezoelectric element and the object under examination. This limitation has restricted their usage. To overcome this, non-contact laser ultrasonics has been developed. Both the generation and detection of ultrasonic vibrations are achieved by laser irradiation (Fig. 1).

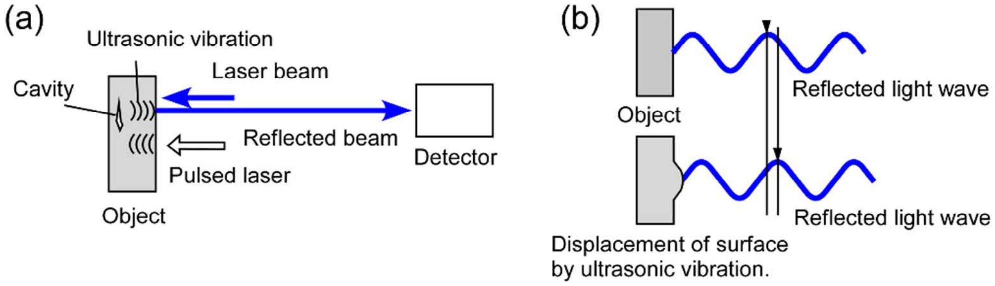

Figure 1. Diagrams of (a) principle of laser ultrasonics and (b) phase shift in reflected light caused by vibration.

By measuring the time it takes for the ultrasonic vibrations to travel inside the specimen and be detected, the thickness and internal structure of the specimen can be determined. In the laser ultrasonic inspection method, it is essential to detect ultrasonic vibrations using light accurately. When an object is illuminated by a laser beam, vibrations can be detected based on changes in the reflected light. The authors have recently demonstrated that laser ultrasonics using a photorefractive flexoelectric (PR-flex) liquid crystal (LC) can achieve high sensitivity and low noise [1]. This system is ideal for portable measurement devices because it uses the properties of LCs to perform measurements without general interferometers, and requires only a straightforward optical system. In this study, laser ultrasonic measurement experiments were carried out using optical setups in which pulsed and detection lasers irradiated opposite sides of an object (counter-optical setup) and the same side of the object (coaxial-optical setup). In both setups, the ultrasonic vibration changes the phase of the reflected beam, which is detected by the change in asymmetric energy exchange. The coaxial setup is suitable for portable measurement instruments to study the internal structure of an object.

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Drop-on-Demand Inkjet Printing of Liquid Crystals and Polymer Composites for Photonic Applications

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Keywords: (Inkjet Printing, Microlenses, Smart Windows, Chiral Reflectors, Additive Manufacturing)

Drop-on-demand (DoD) inkjet printing stands out as a precise, scalable, and cost-effective additive manufacturing technique that enables a plethora of materials to be deposited onto a range of different substrates. Over the past decade, there have been a number of reports that have showcased its potential of printing nematic and chiral nematic liquid crystals (LCs) for various applications such as sensors, printable lasers, and thermally-tunable microlenses. [1-3] In this presentation, we highlight our recent research on inkjet printing of LCs and demonstrate a range of alternative photonics technologies fabricated using this manufacturing process.

The presentation will begin by considering the conditions necessary to print LCs without jet break-up and satellite droplet formation before we show how to fabricate electrically tunable microlenses that exhibit bifocal tuning (Fig. 1a). Using homeotropic surfactants, plano-convex lenses with diameters ranging from 122 µm to 255 µm, resulting in focal lengths for red light (λ = 633 nm) from 228 µm to 463 µm, respectively. Remarkably, these microlenses exhibit bifocal behavior under an electric field without altering the geometric shape of the lens. Furthermore, we present spatially patterned polymer dispersed LC films fabricated using this printing process and demonstrate new smart window technology featuring logos and images that can be made to disappear with the application of a voltage (Fig. 1b). The presentation concludes with a demonstration of colored reflector arrays (Fig. 1c) along with an outlook to the future for this printing technique.

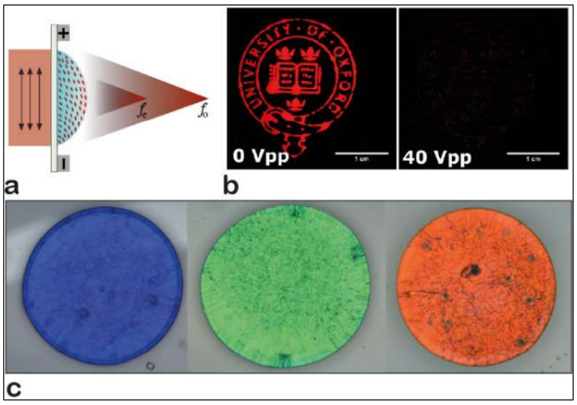

Figure 1: a) Schematic illustration of a microlens showing focal length tuning. b) a printed polymer dispersed liquid crystal film in the form of the University of Oxford emblem that is visible in the absence of a voltage but disappears with the application of voltage. c) printed chiral reflectors with red, blue, and orange colors. [4-6]

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Efficient diffraction gratings based on geometric phase chiral liquid crystal

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Keywords: diffractive optics, chiral liquid crystal, geometric phase, spectrometer, 2D grating

Chiral liquid crystal self-organizes in a periodic helical structure with a photonic band gap for circularly polarized light. For a certain wavelength interval, this results in a reflectivity of over 90% for a layer with thickness more than 3 µm. By using patterned photoalignment at the substrates that enclose the liquid crystal, the orientation of the helical axis and the reflection properties can be designed with a high degree of freedom. The azimuthal angle of the liquid crystal director at the surface of the layer determines the geometric phase for reflected light. With a well-chosen geometric phase distribution, arbitrary lens functions can be realized.

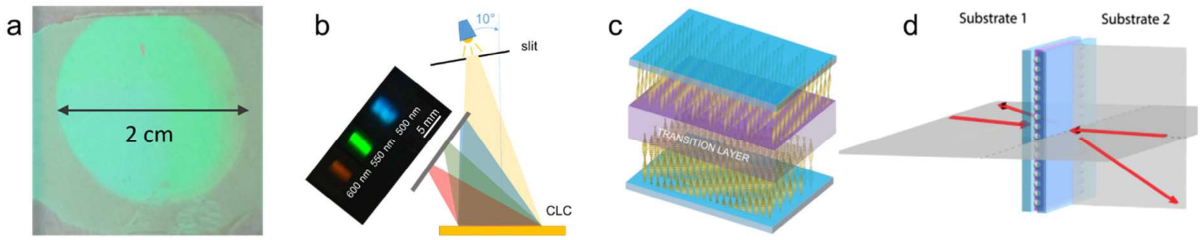

Figure 1: a) Image of a chiral liquid crystal flat optical component with spectrometer functionality; b) Principle of a single component spectrometer; c) chiral liquid crystal layer between two substrates with alignment patterns with perpendicular periodicity; d) Asymmetric diffraction from two sides: in a horizontal and a vertical plane.

Geometric phase gratings with chiral liquid crystal have been used to realize a number of optical components. One example is a spectrometer based on a single liquid crystal component [2]. The flat optical diffractive element at the same time diffracts and focuses light that is incident from a rectangular slit onto a linear detector as illustrated in Fig. 1 (a,b) . A second example is a device with asymmetric diffraction properties: at one side, light with normal incidence is diffracted horizontally, while at the other side light is diffracted vertically, as illustrated in Fig. 1 (c,d). Other components using chiral liquid crystal diffraction gratings are under preparation.

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Electrically accessible metastable configurations in photo-aligned liquid crystal cells

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Keywords: photo-alignment, metastability, electrical tunability, diffractive optical elements

To design functional liquid crystal (LC) components, nowadays a lot of attention is given to the use of patterned surface alignment. High-resolution photo-alignment patterning enables accurate steering of the LC self-organization in the bulk, and the use of different LC materials allows to control the optical properties and tune the stimuli-responsive device behavior.

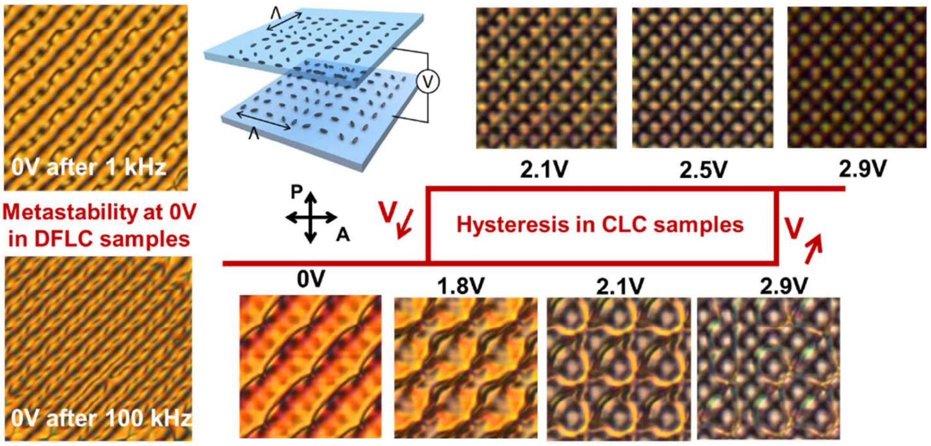

Figure 1: POM images of cells with crossed assembly of rotating alignment patterns: metastable states at 0V in DFNLC (left) and hysteresis switching in CLC cells (right).

In nematic LC cells, a crossed assembly of rotating planar alignment patterns on the substrates (Fig. 1) can either lead to a web of twist disclinations or to a defect-free configuration with strong out-of-plane reorientation. In the latter case, the surface-induced twist conflict is resolved by introducing regions with vertical director. To avoid the need for disclinations, symmetry-breaking takes place and a LC superstructure is formed with lower periodicity than the boundary conditions. We have shown that this anchoring pattern in combination with long-pitch CLC leads to the formation of two different topological states at high and low voltages (Fig.1, right). Switching between both occurs via a hysteresis loop and the resulting optical properties can be steered by adjusting the surface alignment period, the cell thickness and the amount of chirality in the LC [1]. Recently we also demonstrated that by using dual frequency (non-chiral) LC, reversible switching can be obtained between a disclination-free periodic structure and two configurations containing disclinations (Fig. 1, left). Depending on the voltage treatment, three different topological states can be obtained that are all metastable at 0V. The relative stability of these states depends on the surface anchoring period, the LC material and the cell thickness.

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Electrically controlled liquid crystal-based varifocal microlens array on flexible substrates

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Keywords: Liquid Crystals, Norland Polymer, Microlens Array, Tunable lenses

In modern display technology, flexible microlens arrays (MLA) are emerging devices that can be integrated with curved displays for three-dimensional(3D) visualizations [1,2]. Liquid crystals (LCs) have revolutionized the field of lenses, which have recently been utilized to develop tunable microlens arrays [3]. In this work, we developed an electrically controlled varifocal MLA on flexible Polyethylene Terephthalate (PET) substrates by infiltrating the LC in polymeric concave lenses. The polymeric MLA is formed on the PET by exposing the NOA65 using UV light through a circular dot array photomask. The focusing and imaging characteristics of the LC-MLA are studied using a standard test chart. The LC microlenses focus the light beam at their focal plane. When a high voltage is applied, the refractive index of the LC (1.53) and NOA65 (1.524) becomes almost equal; therefore, the MLA behaves as a transparent medium, as shown in Figure 1. The variation of focal length with applied voltage is studied. The elemental image array of a 3D object is captured from different perspectives using a curved and flat LC-MLA, and the comparison shows that the curved pickup of elemental images exhibits more depth perspective than the conventional pickup methods. The mathematical analysis of the LC-MLA is also performed using the MATLAB platform, which shows consistency with experimental results.

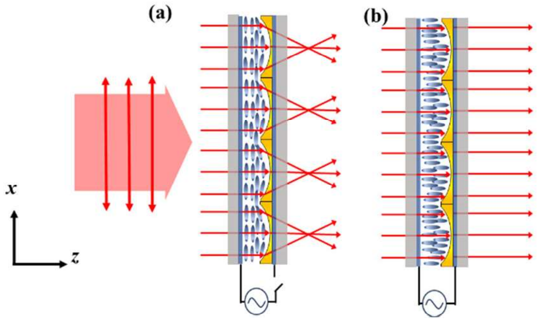

Figure 1: (a) LC-based microlens array (b) transparent state when voltage is applied.

Acknowledgements: The authors thank Indian Institute of Technology Delhi, New Delhi, and Defence Research & Development Organization, India (Grant no. FTM/03/3203/P/01/JATC-P2QP-01) for project funding and research facilities. The authors acknowledge CSIR-HRDG Government of India for senior research fellowship [Grant no. - 09/086(1330)/2018-EMR-I].

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Electromagnetic band structure of a rotating structurally chiral nematic

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Cholesteric, optical properties, band structure, discrimminatory filter

Abstract

We consider an cholesteric liquid crystla which is such that its dielectric tensor twirls uniformly along the helix axis. Our aim is to research the optical band structure when the medium is rigidly rotating around the helix axis to a fixed constant frequency. Starting from the Maxwell equations, we establish a set of equations for the electric and magnetic fields. These equations allow us to calculate the band structure written in terms of the externally imposed rotating frequency. We find that the band structure strongly depends on the rotation frequency, and we show that backward and forward modes propagate differently giving rise to a bias for forward waves We state our concluding remarks.

Acknowledgements: We acknowledges partial support from Papitt Dirección General del Personal Académico UNAM grant IN100921.

Harnessing Molecular Orders Induced by Interfacial Interactions of Microdroplets for Bio-inspired Intelligent Materials

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Keywords: liquid crystals, molecular alignment configuration, smart microparticles, Microdroplets

The programmable responsiveness and functionality of liquid crystal (LC)-based materials, such as shape morphing and color change under external stimuli, have attracted broad interest in designing intelligent materials. Methods such as mechanical stretching and shearing, surface alignment, and field-assisted alignment have been developed to program the order of LC molecules for the desired responsiveness. However, the huge size mismatch between the nanometer-sized LC mesogens and the targeted macroscopic objects calls for questions about how to delicately control molecular order for desired performance. In nature, the responsive materials are built from molecules that assemble into microdomains, and the materials are constructed by using the microdomains as active components. Inspired by this hierarchical design strategy, LC microparticles are used to bridge the gap between molecular scale and macroscopic scale for the synthesis of intelligent materials based on LCs. The molecular order of LC molecules inside microdroplets is tuned by adjusting the surface anchoring effect governed by surfactants, which can be combined with chiral dopant addition to generate microdroplets with reflective structural colors. The alignment configuration can be fixed by polymerization for the synthesis of microparticles with reversible shape-morphing properties, and nanoparticles can be incorporated to introduce new functionalities. The shape-changing microparticles are exploited to program shape-morphing behaviors of inactive elastomer films via magnetic field-guided embedding and fabricate microarrays with switchable optical polarization via template-assisted embedding. Microparticles capable of color switching can be used for camouflage and information encryption. The molecule-microparticle-macroscale hierarchical design provides a strategy for designing LC-based intelligent materials, paving the way for various unforeseeable applications.

Acknowledgements: National Natural Science Foundation of China

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Hierarchical liquid crystal microstructures for multi-degree optical field manipulation

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Keywords: (liquid crystal, helical superstructure, photoalignment, planar optics, geometric phase, vortex)

Vital fields such as supercomputing, constellation satellite & 5G/6G communications, virtual/augmented reality, and holographic displays desire super-large-capacity information processing. Photon informatics exhibits superiorities to electronic techniques due to its intrinsic multi-dimensional and large-scale parallel processing. Thus accurate, efficient, and orthogonal manipulation of the multi-dimensional parameters of light, especially the on-demand tailoring on working frequency and spatial phasefront, is highly pursued. Here, a dynamic polarization photo exposing system is adopted to record the polarization distribution to the spatial orientation of a photoalignment agent, and further guide the self-organization of cholesteric liquid crystals. Via preprograming the initial orientation of the helixes, spatial geometric phases can be arbitrarily encoded to the reflected light in a reconfigurable way. These planar optics exhibit unique properties such as spin dependency and broadband tolerance. Via electrically driving the nano helix of a photopatterned heliconical cholesterics, the reflective Bragg band can be precisely selected in the range from 380 nm to 1550 nm reversibly. Spin-decoupled transflective spatial light modulations are demonstrated in a piecewise-twisted anisotropic monolayer. Besides the wavelength selection and geometric phase modulation, spatial amplitude modulation and spin reversion can be further expected. It enriches the fundamental understanding of soft matter photonics and may upgrade optical informatics.

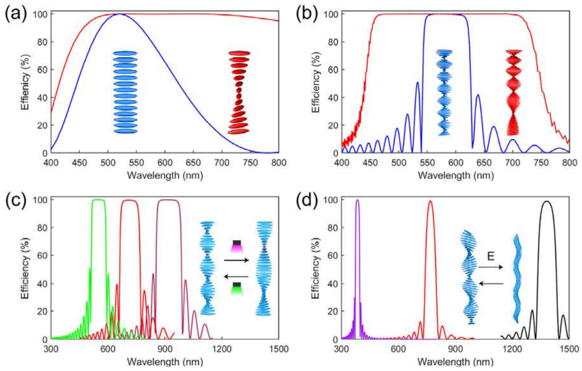

Figure 1: Simulated dependencies of phase modulation efficiency on wavelength of various LC planar optics.

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Inorganic 2D material liquid crystals for deep UV light modulation

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Keywords: liquid crystals, 2D materials, deep UV light modulation, inorganic materials, stability.

Liquid crystal (LC) is one of fundamental optical materials with their birefringence controllable by external magnetic/electric stimulus. Modulators based on organic LCs have shown desired modulation capability with an annual global market of >100 billion US$, but with challenges of weak sensitivity, material stability, toxicity, and limited light modulation range mainly in the visible to infrared regime. In this talk, I will discuss our recent results of using inorganic 2D materials as LCs. Such inorganic 2D material LCs possess extremely sensitive response to external magnetic or electric field, good stability, and capability to tune deep UV light down to 260 nm which is not possible previously. In addition, such inorganic 2D material LCs can be produced in large quantities with a low cost when start with natural layered minerals.

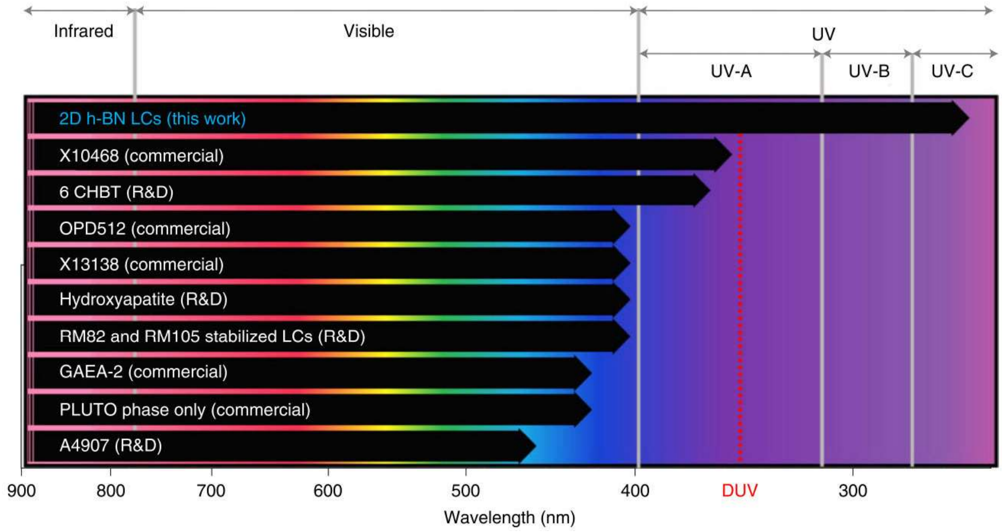

Figure 1. Work range of the established UV light modulators and the 2D h-BN liquid crystal DUV light modulator.

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Investigation of Nematic Liquid Crystal Behaviours when Confined in Stripe Geometries

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Keywords: Nematic; Confinement; Modelling; Defects; Sensing;

Chemically patterned stripes of varying aspect ratios were fabricated on glass surfaces. A hydrophobic surfactant surrounding the stripes allowed confinement of nematic liquid crystals (NLC). The top NLC stripe surface is open to air. A simple model to geometrically describe the cross-section of the confined NLC was derived and compared to an existing, more detailed model[1]; both were compared to experimental data. It has been shown that interference fringes in reflection mode microscopy can be used to find the height of the NLC stripe[2]. This is valid for heights under ~3μm therefore for taller stripes, birefringence colours were used in this work for features with retardation within the range of the Michel-Levy chart. The colours presented differently depending on the surface treatment of the stripe (glass or a rubbed polymer alignment layer). For example, the texture was generally smoother for rubbed samples (Figure 1). The effect of sample rotation with respect to the crossed polarizers for these colours is discussed.

Factors including stripe geometry, LC properties and alignment conditions are discussed. For example, a 'central' defect perpendicular to the rubbing direction was commonly seen in the rubbed case, but not generally on the glass surface (Figure 1). The sign, strength, and frequency of other defects in the texture for both conditions are discussed and compared. As NLC director field changes on addition of analytes is a key detection method in sensors utilizing LC[3], this work can be applied to sensors in the future.

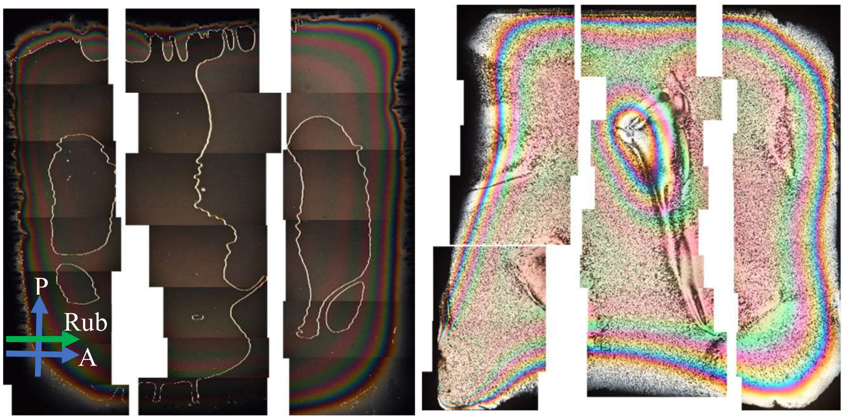

Figure 1: Composite demonstrative tranmission polarized optical microscopy images of 3.52±0.04μL of confined NLC in a ***16x16mm*** *square on (left) rubbed polymer alignment layer with the rubbing direction approx. Aligned with one of the crossed polarisers, or (right) glass surface. The central defect is clearer on the rubbed image, with a more random LC texture for the non-rubbed sample.*

Acknowledgements: *Funding:* EPSRC, UKRI.

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Laser Written Liquid Crystal Tunable Optical Devices

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Keywords: Tunable optics, optical vortex beams, blazed gratings, 3-D printing, two-photon polymerization, direct laser writing.

We present a platform for manufacturing tunable and switchable optics with very simple drive electronics. Two-photon polymerization direct laser writing is an additive manufacturing technique that has been demonstrated to produce micro- and nano-scale features in photoresists. Here, the same process is used to structure the director profile of a polymerizable liquid crystal (LC) in 3-dimensions to form a 3D spatial phase profile. Due to the flexibility of this fabrication process, it has been used to make a wide range of tunable and switchable devices, including diffractive optical elements, lenses, and aberration correctors [1-4]. In this work, we demonstrate the success of this technique for producing tunable phase plates that contain phase discontinuities, specifically, optical vortex beam generators and blazed gratings. We include a range of characterization methods, including polarization optical microscopy (POM), and far-field and interferometric transmission imaging, that demonstrate the effectiveness of these devices for tuning over function (vortex/diffraction order) and operating wavelength. We discuss the scalability of these devices to add greater functionality without the need for excessive and complex drive electronics, and the impact this platform technology could have in the field of optics.

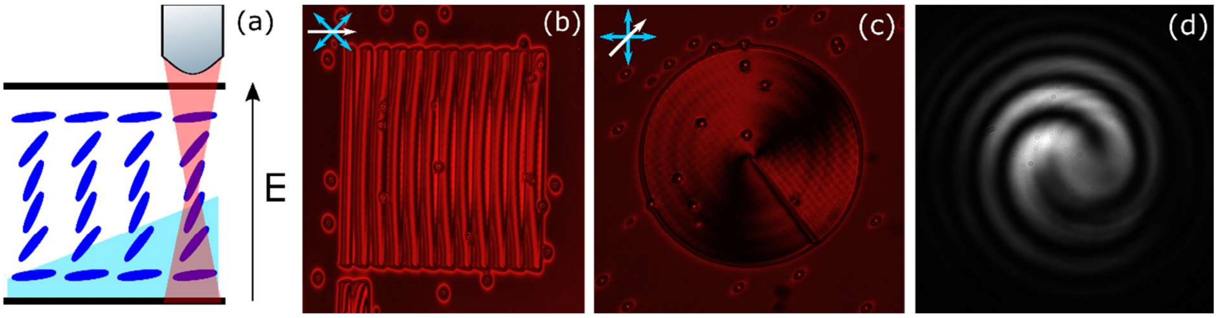

Figure 1: (a) Illustration of fabrication process, (b) POM image of prototype LC laser written blazed grating, (c) POM image of a LC laser written optical vortex beam generator, (d) interferogram produced when the optical vortex beam interferes with a spherical wave.

Acknowledgments: This research was part-funded by Engineering and Physical Sciences Research Council (EPSRC) in the UK: grant EP/R004803/01 (EPSRC Fellowship Patrick Salter), grant EP/R511742/1 for an Impact Acceleration project, and grant EP/T517811/1 (a CASE Conversion studentship award with Merck Ltd. for Camron Nourshargh). This research was also supported by the John Fell Fund (Oxford University Press) and The Royal Society (UK) who provided resources for the laser writing facility.

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Light modulators and displays for green photonics

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Keywords: light modulators, organic photovoltaics, photoactive materials, liquid crystal photonics, liquid crystal materials and techniques

Photonic liquid crystal devices, including flexible thin screens, waveplates, smart glasses or AR/VR systems, typically require an external power to control them. The current challenge is to realize energy efficient and autonomously operated components, by harnessing light to control light. In this talk, a new generation of such optically addressable, photovoltaic driven optical modulators will be presented.

Photovoltaic spatial light modulators (PSLM) are self-activated optical devices that can be used for dynamic glazing, optically addressable spatial light modulators or microdisplays. They contain an organic photovoltaic unit as an integrated power source to drive and control light transmission in liquid crystal modulators [1] and can operate as self-powered devices. The structure of the modulators includes either a planar or a twisted nematic liquid crystal layer and an organic donor-acceptor bulk heterojunction, the latter being in contact with the liquid crystal and also acting as a molecular alignment layer. Under illumination, the photovoltage can be sufficiently strong to partially reorient the liquid crystals and thus change the optical transmittance of the modulator, without requiring an external power source.

The operation of PSLMs can be tailored by the choice of materials and dopants that control clear-state transmittance, spectral distribution of transmitted light as well as response time and stability. While these parameters are mainly controlled by the materials used for PSLMs, other – such as pretilt angle or anchoring energy – are determined by the geometry and the interaction of a particular liquid crystal with the alignment, photovoltaic layers, and substrates. The overall performance of such devices is, therefore, governed by the interplay of a large number of parameters. This applies, in particular, for devices such as PSLMs that combine both liquid crystal and photovoltaic technologies and where it is essential to characterize final, working devices in a non-invasive way. Reliable optical method will be presented that can capture, accurately and in a reproducible manner over a long-time scale, both static and dynamic properties of PSLMs and other liquid crystal devices. In addition, either a single spot or a large area of the PSLMs can be probed, thus allowing us to map [3] spatial changes in pretilt, anchoring, and uniformity of the device across the whole panel of the modulator. This approach aids not only the understanding of the fundamental, physical processes behind photoactive devices, but also in the development of the related, green photonics technologies.

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Liquid-crystal-based terahertz wave modulator

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Keywords: Liquid crystals, Terahertz, Geometric phase, Optics

Terahertz waves have broad applications in fields such as security screenings, non-destructive inspections, and high-speed wireless communication. People expect to achieve terahertz wave switching, polarization control, attenuation, filtering, and even mode encoding and routing like manipulating light. Therefore, achieving efficient, switchable, and multifunctional terahertz modulation has become a key research topic. Liquid crystal is a promising electro-optical material, but terahertz devices based on liquid crystals face a series of challenges and research is not yet sufficient. We propose a terahertz modulator similar to its visible and telecom counterparts and verify its applications in amplitude, phase, polarization and complex wavefront modulation of terahertz wave. We also combine liquid crystals with metasurfaces to fully explore the dynamic electric field manipulation of liquid crystals based planar optics. We use terahertz time-domain spectroscopy to study the liquid crystal integrated metasurfaces, and solve a series of problems of liquid-crystal-based terahertz components, and realize dynamic and efficient terahertz wavefront control.

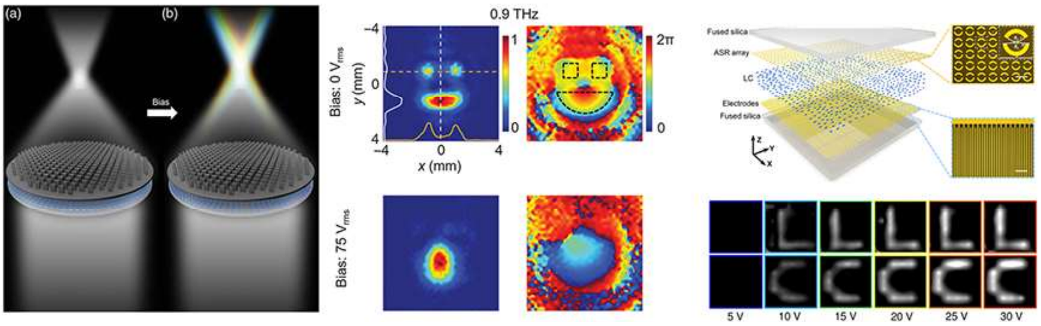

Figure 1: Liquid crystal integrated metalens with switchable chromatic aberration and electrically addressed spatial THz wave modulator.

Acknowledgements: The work was supported by the National Key Research and Development Program of China (2022YFA1203703) and the National Natural Science Foundation of China (NSFC) (62035008).

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Liquid Crystal Elastomer Lenses

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Keywords: Optics, Lenses, Elastomers

Liquid crystal elastomers are weakly crosslinked polymer systems with liquid crystalline order. This gives them the combination of liquid crystalline order with the elasticity of rubber [1-3]. This unique system offers some interesting optical properties due to the liquid crystal anisotropy, whilst also being able to undergo a rubber like elastic response [4]. Utilising formulations of 6OCB, A60CB, RM82, EHA and MBF they can maintain a high optical transparency similar to glass [5]. In this work liquid crystal lenses made from liquid crystal elastomers are discussed utilising a variety of fabrication techniques such as electrode patterning to create flat GRIN type lens, as shown in figure 1.a), or using moulds to shape the liquid crystal elastomer, as shown in figure 1.b). Due to the liquid crystal elastomer lens's polarisation dependence and high optical transparency, the lenses could act as a replacement to conventional calcite lenses or new designs where change can be initiated through thermal or mechanical methods.

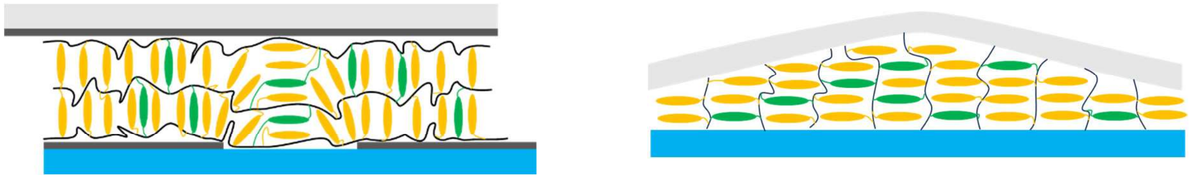

Figure 1. a) Liquid crystal elastomer lens made using a hole patterned electrode between ITO coated PET film and glass. The liquid crystal is represented by the yellow molecules and the green represents the crosslinker. A strong voltage is applied to the system aligning the liquid crystal elastomer so that a gradient can be made in the refractive index, creating a lensing effect. This can then be cured using UV light to maintain the alignment. b) Liquid crystal elastomer lens made using a lens shaped mould. The liquid crystal is represented by the yellow molecules and the green represents the crosslinker. Due to the liquid crystal's birefringence the lens will have two different focal points depending on the polarisation orientation of the input light.

Acknowledgements: The authors would like to thank the University of Leeds and EPSRC for funding (EP/V054724/1)

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Liquid Crystal Speckle Reducers for Laser Display and Imaging Applications

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Keywords: laser speckle, liquid crystals, laser-imaging, laser projection.

Lasers, revered for their exceptional directionality, intensity, and expansive colour gamut, stand as coveted sources for imaging and display applications [1]. However, their coherence, a necessity in optical diffraction-based imaging, produces a spatially distributed granular noise known as speckle, an artefact arising from random contributions of constructive and destructive interference from scattered light [2]. This work presents a solution: liquid crystal (LC) based speckle reducers manufactured from short-pitch chiral nematic LCs, inducing a dynamic scattering mode via electrohydrodynamic instabilities under specific electric field driving conditions [3-5]. To evaluate devices, a characterization system designed to emulate human visual perception has been developed, enabling quantification of the speckle contrast parameter, C, as defined by J. Goodman [2]. Through strategic optimization of device architecture and material composition, incorporating ionic, redox, and zwitterionic dopants [4-6], we achieve a substantial reduction in speckle contrast to an almost imperceptible level ($C = 0.07$) with the devices operating in either a transmissive or reflective configuration. These advancements have the potential to enhance various laser-based projectors, enabling high-quality, speckle-free imagery. Therefore, this presentation will conclude with the demonstration of these LC speckle reducers in a range of diverse applications including microscopy, head-up displays, and laser projection [6] (Figure 1).

Figure 1: (*Left) RGB Laser head-up display demonstrator with i) no speckle reduction, ii) active speckle reduction from a transmissive configuration LC device. (Right) RGB Laser projector demonstrator with i) no speckle reduction, ii) active speckle reduction from a reflective configuration LC device.*

Acknowledgements: N.P.S. gratefully acknowledges the Engineering and Physical Sciences Research Council (EPSRC) UK for financial support through a graduate student scholarship (EP/T517811/1). S.M.M., S.J.E. and M.J.B., gratefully acknowledge financial support from the EPSRC (UK) through project EP/W022567/1.

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Optical Switch Based on Polymer-Stabilized Dual-Frequency Liquid Crystal Comprising a Thermally Responsive Chiral Dopant

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Keywords: Thermoresponsive chiral dopant, Dual-frequency liquid crystal, Polymer-stabilized liquid crystal

Research on optical switches has received much attention in recent years [1]. In this study, we developed an optical switch that can achieve stable states within a certain range of transmission by taking advantage of the unique property of a chiral dopant (TCD) whose helical twisting power (HTP) decreases, changing from the right handedness to the left, with rising temperature (*T*) in a vertically aligned, polymer-stabilized dual-frequency liquid crystal (DFLC) cell. As shown in Fig. 1(a), the absolute value of the net HTP of a chiral-dopant duo (S811 and TCD) in pure DFLC (HEF951800) increases with increasing *T*. At *T* below 32 °C, the HTP of the chiral molecules cannot compete with the vertical alignment effect from the polymer, resulting in the polymer-stabilized LC remaining in the homeotropic (H) state. On the contrary, when *T* exceeds 48 °C, the helical strength becomes significantly large so that the system enters the scattering (S) state. Because of the two competing (i.e., winding and straightening) effects, transmission can be regulated by applied voltage and the transmission level persists after turning off the voltage. Figure 1(b) depicts detailed transmission tuning at 35 °C, between the initially highest transmission (at 0 V_{rms}) and lowest transmission induced by 50 V_{rms} at 200 kHz; the spectral transmission level then increases with the increase in applied voltage at 1 kHz. Figure 1(c) shows the reproduceable spectral data obtained after voltage manipulation of 150 times, manifesting the switch between two arbitrary transmission levels.

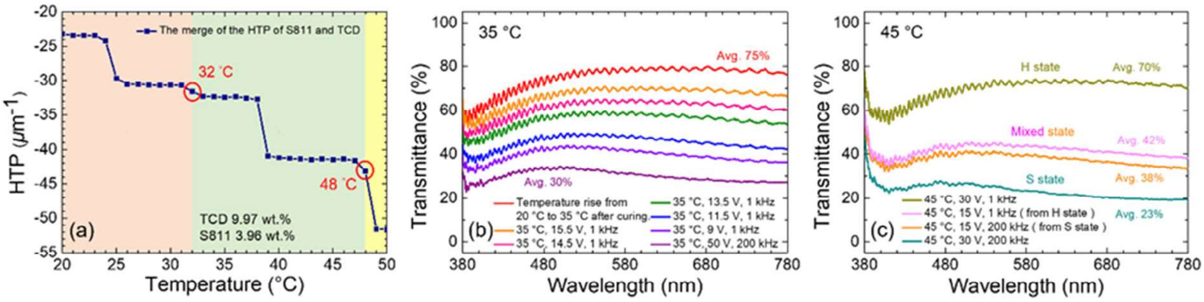

Figure 1: (a) Temperature-dependent HTP of mixed S811 and TCD in DFLC; (b) transmission spectra of the polymer (4 wt.%)-stabilized DFLC in various AC-voltage conditions at 35 °C; (c) transmission spectra for different applied AC voltages at 45 °C.

Acknowledgement: National Science and Technology Council, Taiwan (112-2112-M-A49-031).

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Photoinduced modification of cholesteric structure with tangential-conical boundary conditions

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Keywords: cholesteric, conical anchoring, photosensitive dopant, orientational structure

Cholesteric liquid crystals (CLCs) are optically active media that are widely applied in science and technology. The orientational structures and optical properties of the devices based on cholesterics mainly depend on the boundary conditions and the ratio of space value d to helix pitch p (length at which the director rotates through 2π-angle). Recently, CLCs with light-controlled helix pitch have been actively studied [1] since they allow developing systems with a smooth change in the twist angle of the structure under continuous variation of helix pitch. Photosensitive CLC layer with tangential-conical boundary conditions [2] is considered. Nematic mixture LN-396 doped with a left-handed chiral additive S5011 (Macklin) and a right-handed photosensitive chiral dopant cChD (CNM Institute, NAS of Belarus) was used. The transformation of CLC structures have been studied by polarizing microscopy. Initially, the structure with linear defects was formed in CLC layer (Fig. 1a). These defects are located at the surface with conical anchoring, and the director near the defect is parallel to it. When irradiated with light, the helix pitch varies from 16.9 µm to 88.0 µm, which leads to a smooth change in the structure twist angle from –380° to –70°. This causes the defects to become unstable. The defects are transformed in two stages, and at each stage the pairs of reverse points are formed moving in opposite directions along the defect lines (Fig. 1b,c). As a result, the continuous linear defect is transformed into a line with the reverse points located at each 180°-bend.

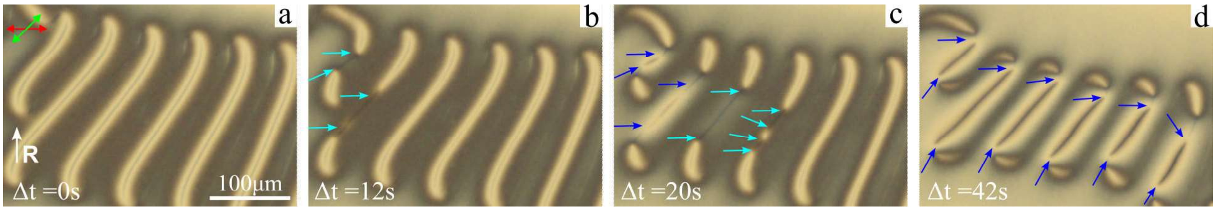

Figure 1: Photos of photosensitive cholesteric layer in crossed polarizers (polarizer and analyzer are shown double red and green arrows) in the initial state (a) and taken in 12 (b), 20 (c) and 42 (d) seconds after switching on the microscope lamp. The director orientation **R** on the substrate with tangential anchoring is shown by a single white arrow, and the turquoise and blue single arrows indicate the reverse points for the first and second stages, respectively.

Acknowledgements: the research was funded by Russian Science Foundation, Krasnoyarsk Regional Fund of Science and Technology Support, Government of the Krasnoyarsk Territory, Grant No. 24-12-20007, https://rscf.ru/en/project/24-12-20007/

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Polarization dependency of varifocal lenses via nematic liquid crystals

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Keywords: LC devices, namatic liquid crystals, varifocal devices, lenses, polarization dependency

Varifocal lenses via nematic liquid crystals(LC) was proposed in 1979[1]. To remove polarization dependency of intrinsic properties of LC phase modulation while maintain large phase shift, the double-layered structure of varifocal LC lenses is typically adopted [2-8]. The mechanism is to have two eigen-polarizations of light accumulate same phase shift after unpolarized light propagates through two identical homogeneous aligned LC layers with mutually orthogonal alignments. However, the corresponding polarization dependency of the double-layered structure of the varifocal LC lenses is not studied in detail. In this paper, we would like to tackle this topic to understand how the polarization of incident light propagates in the double-layered structure and the corresponding limitation. We hope this study would provide optical perspectives to researchers to understand polarizer-free varifocal LC lenses and inspire novel design of polarizer-free LC lenses.

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Real-Time Hyperspectral Imaging is Enabled with a Thin Liquid Crystal Spectral Modulator and Deep Learning Algorithm

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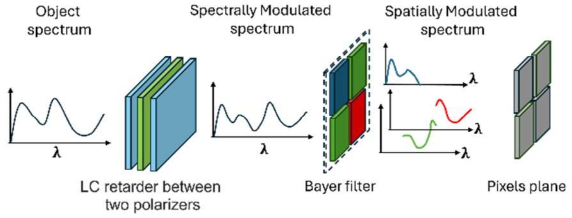
Keywords: Hyperspectral Imaging, Deep Learning, Computational Spectroscopy,

Spectral imaging holds significant promise across various fields, but traditional methods using LC tunable filters have faced limitations in terms of flexibility, speed, and cost-effectiveness. The emergence of computational spectral imaging systems, driven by advancements in Deep Learning algorithms, has brought about a transformative shift in this domain. These systems leverage the power of machine learning to reconstruct spectral information from captured data, offering enhanced performance and flexibility compared to traditional methods [1]. However, despite their potential, computational spectral imaging systems still face challenges that limit their widespread accessibility.

In this study, we demonstrate a novel method for acquiring high-resolution hyperspectral information using an LC retarder and a standard smartphone camera. Our system utilizes a single pixel 8μm LC modulator in conjunction with a tailored deep learning algorithm, calibrated to ensure real-time, high-quality performance. In our approach, the LC modulator induces spectral modulation of the object spectrum at specific voltages. This modulated spectrum is then filtered through the built-in Bayer filter (RGBG) of a CMOS camera, introducing spatial modulation where each pixel captures a distinct portion of the spectrum (see figure). Notably, our method requires only 7 different voltage settings, significantly fewer than the traditional computational spectroscopy which typically necessitates over 100 settings. From a mathematical standpoint, the spatial modulation results in a substantial reduction in the dimensionality and complexity of the inverse problem, facilitating a more reliable recovery of the complete spectral information. By employing faster LC modes and specialized driving schemes, our approach can even enable hyperspectral video capture. This innovative methodology holds the potential to revolutionize spectral imaging and liquid crystal technology applications. Our ultimate goal is to integrate an LC retarder with a smartphone camera, making this technology accessible to the general public. This advancement could pave the way for transformative applications in telemedicine and other fields.



Acknowledgments: The project is supported by the Ministry of Science and Technology.

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Sunlight-Fueled Broadband Tunable 3D Blue Phase Photonic Nanostructure in Molecular-Motor-Based Chiral Nematics

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Keywords: blue phase, molecular motor, tunable, photonic band gap

ABSTRACT: At present, the main ways to control the crystal structures of blue phase (BPs) are by means of changing temperature, applying external voltage, and light irradiation. In 2005, Chanishvili et al. were the first to add achiral azobenzene materials to BPLC, which enabled the element to rapidly switch the reflection band when irradiated by UV light and showed the possibility of remote control [1]. However, the contrast of helical twisting power (HTP) between cis-trans isomers based on azobenzene materials is little. So, the light-induced reflection band shift is limited to 100 nm, which obviously cannot fulfill the needs of display technology. In this work, we introduced a sunlight-driven, ultra-broadband photo-tunable blue phase liquid crystal device, where the adjustable range of the reflection wavelength is significantly expanded through adding chiral overcrowded alkenes, known as molecular motors. Molecular motors were first developed by Dutch chemist B. L. Feringa and his team [2]. Since the fluorene group in the chemical structure of molecular motors is structurally compatible with the biphenyl core of the LC host E7, the HTP it provides to LC molecules is enough to form BP. Experimental results present that clean, reliable, and renewable solar energy stimulation can induce the gradual change of BP into a structure with longer pitches, leading to a red-shift of photonic bandgap (PBG) across the entire visible region without phase transition. Therefore, the device can be precisely regulated to certain wavelength by controlling the UV light intensity at room temperature. In terms of applications, low-energy-drive (by sunlight) and the ultra-broadband (470 nm~770 nm) operating range greatly enhance the performance of optical components. With these horizons, the device is expected to have potential applications in light switches, laser tuning, or reflective displays.

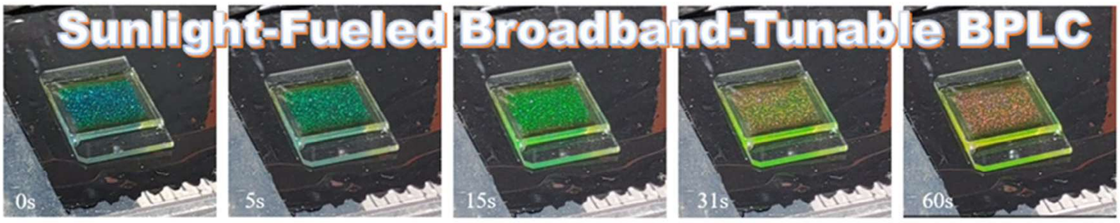

Figure 1: Under sunlight irradiation, the reflective color of molecular-motor-based BP continuously changes from blue to red.

ACKNOWLEDGEMENTS: The authors would like to thank the National Science and Technology Council (NSTC) of Taiwan for financially supporting this research under Grant No. NSTC 112-2112-M-006-021 & NSTC 112-2221-E-006 -168 -MY3.

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Temperature Effect on the Wavelength Shifts of Near-Infrared Defect Modes in a Photonic-Crystal/Liquid-Crystal Structure

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Keywords: Photonic crystals, Nematic liquid crystals, Defect modes, Near-infrared devices.

Photonic crystals (PCs) have been widely discussed and intensively studied in the scientific community. In particular, the combination of liquid crystals (LCs) and PCs has been applied and developed through the outstanding design of injecting a LC material as a defect layer into a PC structure. We have developed a unique methodology to improve the stability and accuracy for atypical micro near-infrared (NIR) spectroscopy involving a PC/LC structure [1]. By conducting experimental measurement and simulation, we first investigated the ordinary and extraordinary refractive indices (n_o and n_e, respectively,) and the resulting birefringence ($n_e - n_o$) in a nematic LC in the NIR region, with a focus on the temperature (*T*) effect as shown in Figs. 1(a) and (b). For the said PC/LC structure, the experimental results indicate that defect-mode peaks in the photonic bandgap blueshift by varying degrees as *T* rises, as illustrated in Fig. 1(c). Grasping the temperature effect and the resulting spectral behavior of the defect modes for four-channel wavelength scanning solves the need for temperature control of the PC/LC cell integrated with a Z-block prism in the core module for an atypical NIR spectrometer.

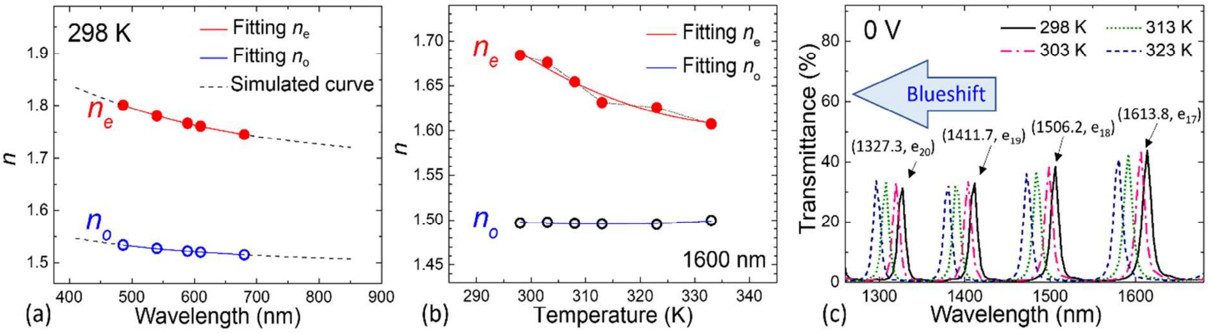

Figure 1: (a) Dispersive refractive indices n_e and n_o in the nematic LC for the defect layer in the hybrid photonic structure; (b) *T*-dependence of birefringence of the LC at the NIR wavelength of 1600 nm. (c) Transmission spectra of a LC layer sandwiched between two identical dielectric mirrors exhibit four blueshifted defect-mode peaks at elevated temperatures without applied voltage.

Acknowledgements: National Science and Technology Council, Taiwan (111-2112-M-A49-033; 112-2112-M-A49-031).

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The added value of liquid crystal-based responsive polymers in photonics, sensing and cryptography

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Keywords: liquid crystalline network, polymer stabilized liquid crystals, photonics, cryptography, reconfigurable functions

Advanced multifunctional integrated photonic and cryptographic hardware demands for reconfigurable materials that can efficiently modulate light propagation. To this end, polymer stabilized liquid crystals and liquid crystalline networks thanks to their large reconfigurable birefringence and shape-changing behavior [1], enable the fabrication of photonic structures whose properties can be dynamically modulated by light or temperature changes.
In this contribution, I will highlight the role of responsive materials for tuning the optical properties of 3D printed photonic microstructures and highly secure cryptographic primitives.

4D nano structuring (3D design with well-defined temporal deformation), achieved by photo-polymerization with direct two-photon laser writing (TP-DLW), has led to various tunable photonic structures: from a 2D diffractive grating structure for optical beam steering [2] to a 3D deformable photonic crystal with sub-diffraction limited resolution [3], from polarization colour pixels for solvent sensing to hidden micro tags that can be unveiled under proper stimuli [4]. On the other hand, when liquid crystals are dispersed in a polymer matric, they form a disordered ensemble of micro droplets that scatter light differently depending on their alignment. Taking advantage of the spatial light control of the birefringence of the disordered media, we demonstrate a multilevel and multiuser generator of cryptographic password [5].

Through the combination of the customizable chemical and physical properties of liquid crystals and 3D engineered photonic structures, we are investigating dynamic, reactive yet deterministic and reliable devices that can open up new advanced technological solutions.

Acknowledgements: The authors acknowledge the support funding PNRR PRIN 2022 "Multi-step optical encoding in anti-counterfeiting photonic tags based on liquid crystals PHOTAG", (project number: 2022T3B4HS) and the Next-Metrology Project #13 LCE-Sense.

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Thermo-Optic Adaptation in Liquid Crystal Smart Windows with a Thermoresponsive Handedness-Changing Chiral Agent

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Keywords: Dual-frequency liquid crystals, Smart windows, Crossover frequency

Research on smart windows that respond to light or temperature changes has significantly advanced in recent years. Photochromic smart windows mainly rely on the integration of photosensitive materials [1], whereas thermochromic counterparts employ phase change substances or incorporate thermally responsive materials [2]. Many previous endeavors on the latter have encountered challenges, such as inability to regulate the transition temperature or requirement of high operating voltage. In this work involving a dual-frequency cholesteric liquid crystal (CLC) doped with a black dichroic dye, we achieved high transmission in the homeotropic (H) state and low transmission in the fingerprint (FP) texture, and successfully developed a normal-mode smart window with tunable transparency at various temperatures by exploiting the chirality cancellation of chiral dopants as shown in Figs. 1(a) and (b). In addition, when an AC voltage of a specific frequency is applied, the CLC molecules exhibit negative dielectric anisotropy at lower temperatures and positive dielectric anisotropy at higher temperatures. As a result, we successfully fabricated a reverse-mode smart window with low transmittance in the Grandjean planar (P) state at lower temperatures and high transmittance in the H state at higher temperatures as shown in Fig. 1(c).

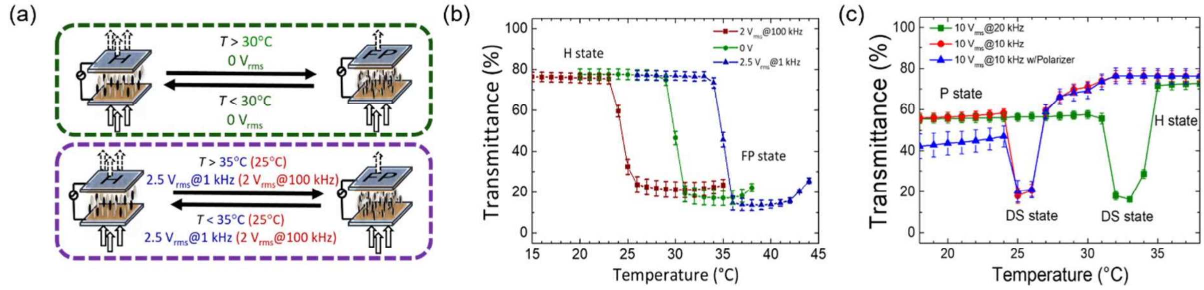

Figure 1: (a) Schematics of passive controls in the normal mode and (b) average transmission as a function of the ambient temperature at various applied voltage conditions for adjustable switching temperature. (c) Transmission spectra in the reverse mode under different voltage and temperature conditions with and without the use of a polarizer.

Acknowledgements: National Science and Technology Council, Taiwan (112-2112-M-A49-031).

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Two-dimensional self-organized liquid crystal photonic potential based on a lattice of torons in an optical microcavity

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Keywords: optical microcavity, torons, self-organized photonic potential

Photonic crystals featuring optical anisotropy have lately become the focus of extensive research. The combination of band structure engineering and birefringence allows for control over the polarization and spin-orbit coupling of light [1]. This leads to the observation of phenomena such as the optical spin Hall effect and spin-directional propagation [2].

Here, we demonstrate an optical microcavity with an embedded well-organized lattice of liquid-crystalline micrometer-sized torons (cholesteric bubbles), which are doped with light emitters. The resulting hexagonal lattice (Fig.1a) provides a photonic potential that confines light. The direct consequence of the periodic confinement is a band structure that shares the symmetry of the photonic crystal (Fig.1(b,c)). TE-TM splitting originating from the microcavity mirrors and the optical activity of the liquid crystal lead to a unique polarization of the bands (Fig.1d). The presence of light emitters in the structure enables laser emission from lattice nodes. Due to the internal structure of torons, the laser emission carries a non-zero orbital angular momentum.

The proposed platform paves the way toward the integration of liquid crystal optical microcavities and self-organizing two-dimensional photonic potentials. The tunable band structures and phenomena related to topology and strong light-matter coupling might be milestones for future discoveries.

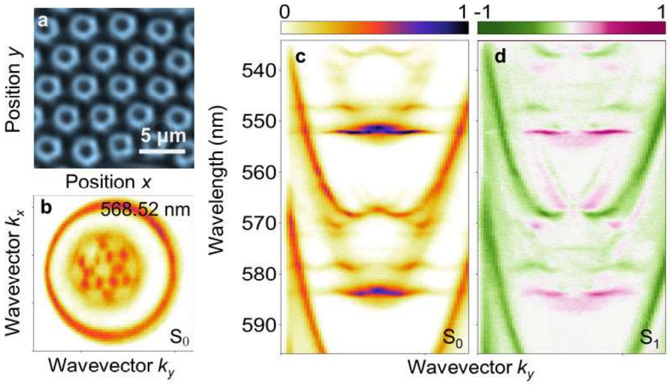

Figure 1: (a) Polarized optical microscopy photograph of the torons lattice (b) Momentum-space image collected for 568.5 nm reveals the symmetry of the photonic crystal. Angle-resolved PL spectrum of (c) total intensity and (d) Stokes parameter S_1. The strong polarization dependence of the photonic bands is well visible.

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Two-step photo-alignment to control the tilt angle of nematic liquid crystals

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Keywords: liquid crystals, photo-alignment, optics

One of the challenges of aligning nematic liquid crystals is to achieve a spatial control of the out-of-plane (tilt) angle. However, this precise control is critical to developing electro-optical devices and programmable origami. We demonstrate a simple method to obtain three-dimensional control of the director field and in particular a spatial control of the tilt angle. The method can be easily implemented in most laboratories and it is based on a two-step photo-alignment process. In the first step, we use polarized light to orient the director on a plane. In the second step we use unpolarized light of a prescribed dose to set the out-of-plane orientation. The method enables smoothly varying orientational patterns with sub-micrometer precision. We demonstrate the method fabricating a gradient-index lens with a parabolic refractive index profile, which remains stable without the need for external electric fields. We characterize the lenses' focal length and sensitivity to light polarization. Our findings pave the way for developing next-generation photonic devices and actuated materials, with potential applications in molecular self-assembly, re-configurable optics, and responsive matter.

Acknowledgements: BSF 2018380, NSF DMR-2104747

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Unravelling Topological Domains in a Nematic Liquid Crystal Pi Cell

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Keywords: Topology, Bistability, Pi Cell, Temperature Sensors, Fast Electro-optic Shutter

Nematic liquid crystal (LC) Pi cells, constitute an important category of devices with potential in applications that demand a rapid switching process. Line singularities known as disclinations play an important role in the understanding of the topography and electro-optic phenomena in LC technologies and there are a number of different topological regimes in a Pi cell. Manipulating these singularities and defects in a precise and controlled way can unlock new functionality and electro-optic behavior for a range of applications including tunable lasers and beam generators for optical communications [1].

This presentation explores the concept of manipulation of the domain regions in a nematic Pi cell through the control of nucleation and growth. We then propose potential applications based on this approach. Utilizing a combination of reactive mesogens and an optical projection system imprinting is achieved that forms spatial patterns of a polymer network in the pi-cell that locks-in various topological states. By modulating the voltage, distinct states with varying boundary conditions are generated, establishing a mechanism to impede nucleation and growth by polymerizing different topological regimes inside the LC device. This results in the creation ofa fast shutter that switches between the twist state and the bend state with the ability to indefinitely remain in these states. Separately, bistability within the LC device is achieved by varying the temperature and reapplying a voltage in this locked-in regime, offering potential applications in the development of temperature-sensitive labels for transporting biological molecules, for example. Furthermore, by employing different combinations of topologies to lock in the director states, a bistable LC device responsive to voltage is created.

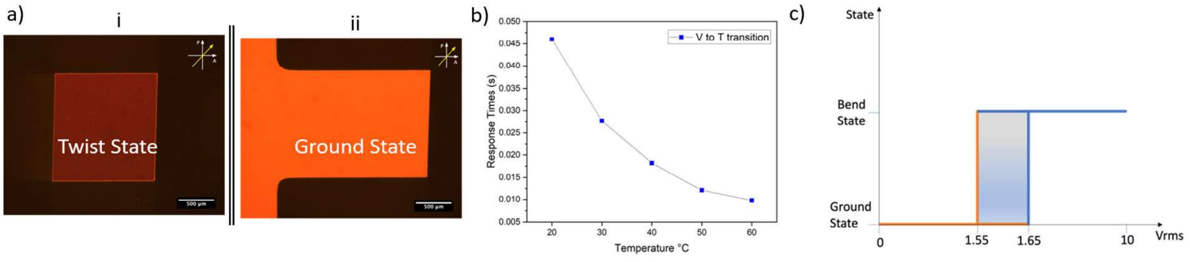

Figure 1: a) Polarized Microscope Images of the device at 0V showing i) the shutter created remaining in the twist state and ii) the other bulk of the LC nucleated to the ground state b) The response times with different temperatures of this fast shutter c) Bistability with voltage creating a hysteresis loop of states.

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D3

Actuators and haptic devices

3D Printing of Liquid Crystal Elastomers for Photo-Thermal Actuation

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Keywords: soft robotics, liquid crystal elastomers, additive manufacturing, actuation.

Soft robots are a type of robotic system constructed with flexible materials, enabling them to adapt to, and interact with, their environment in a versatile and human-friendly manner, offering an alternative to traditional rigid robots [1]. Liquid crystal elastomers (LCEs), smart materials with the ability to undergo reversible shape changes in response to external stimuli, enable the creation of highly flexible and responsive robotic structures [2]. The integration of 3D printing with LCEs in soft robotics allows for precise fabrication of intricate and customizable structures [3].

Here, we explore the use of 3D printed LCEs with photo-thermal actuation at the water/air interface, for realizing a soft robot that mimicks a frog through its jumping motion. Specifically, we made inks of RM257-based and C6BAPE-based oligomers, as well as mixtures thereof, to determine the composition with the most suitable printability, which still allowed for alignment, during the extrusion-based 3D printing. The actuation of 3D printed rectangles with different numbers of layers was systematically compared. Graphene oxide was added to the ink with the aim to use photothermal actuation when the 3D printed structures were illuminated with near infrared light.

The next step forward will be to 3D print a frog-like shape, by combining a passive polydimethylsiloxane ink for the body and an elastomer-based ink for the legs, with the goal to obtain a soft robot which can move at the water/air interface.

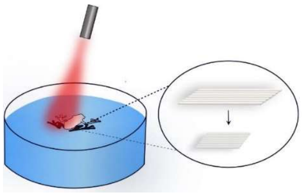

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Figure 1: Photothermal actuation of 3D printed soft robotic frog at water/air interface

Acknowledgements: This work was supported by the Independent Research Fund Denmark (DFF-FNU).

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Fast, high-resolution 4D printing of liquid crystal microactuators

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Keywords: liquid crystal networks, microactuators, 4D printing, dual-wavelength volumetric micro-lithography

4D microactuators are an exciting class of micro-objects made of stimuli-responsive materials. Particularly promising, actuators based on liquid crystal (LC) networks and elastomers (LCNs and LCEs) are capable of programmable, complex, and reversible shape deformations triggered by environmental changes, with applications ranging from microrobotics to smart microstructured haptic surfaces. However, 4D microfabrication at a reasonable speed and resolution remains challenging, hindering both research and large-scale manufacturing. In this work, we for the first time adapt the novel technology Dual-Wavelength Volumetric Micro-Lithography (DWVML) to LC polymers to overcome these existing challenges.

DWVML uses digital light processing and microscopy optics to rapidly print (up to 100 mm^3 h^{-1}) 3D microstructures layer by layer (in contrast to TPP-DLW), over large surface areas, with 100 nm resolution thanks to the employment of localized polymerization photoinitiation and photoinhibition (Figure 1A). Crucial for LCs, in contrast to the majority of microfabrication methods (soft lithography, stereolithography, etc.), many conventional LC alignment methods are compatible with DWVML since printing is done in the cells widely used in LC research.

In our presentation at the ILCC conference, we would like to introduce DWVML to the international liquid crystal community and share out first results, including discussion of DWVML-compatible LC photoresist development and its application to producing arrays of several thousand LCN micropillar actuators in seconds (Figure 1B). An LCN membrane with tuneable micrometre-sized pores will be also demonstrated as a simple application example.

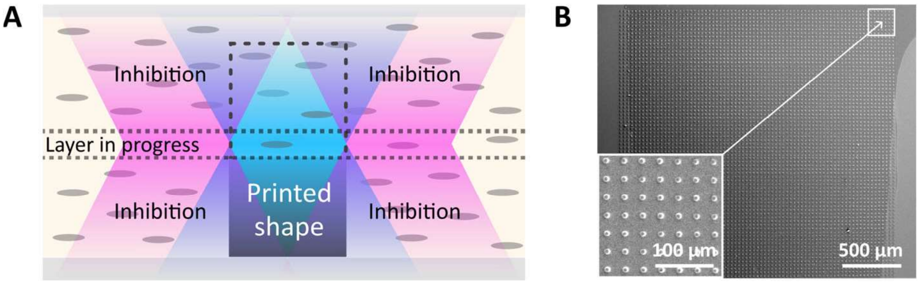

Figure 1: A. DWVML-printing process: a blue image of a layer of a microstructure (e.g. a pillar) is projected in a cell filled with LC photoresist containing a blue light-responsive photoinitiator. UV light is projected around the layer to activate a UV responsive inhibitor and confine polymerization. B. Array of 75x75=5625 LCN micropillars printed with DWVML.

Acknowledgements: This work is financially supported by the Dutch Ministry of Education, Culture and Science (Gravity Program 024.005.020 – Interactive Polymer Materials IPM).

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Human Interactive Liquid Crystal Fiber Arrays

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Keywords: liquid crystal elastomers, fiber actuators, human interactive materials, device integration, remote haptics

This paper presents novel interactive liquid crystal fiber arrays that can actuate in a way perceptible by human touch. The fibers are actuated via a computer interface, enabling precise control over actuation direction, magnitude, and frequency. Unlike conventional methods, this novel technique initiates the actuation at the base of the fibers, which is enabled by fabricating the fibers directly onto an electrical circuit. Fiber actuation is achieved by localized addressing of a radially aligned segment. This induces reduction in the scalar order parameter and leads to deformation of the fiber base, causing bending towards the activated region. Simulations validate this actuation mechanism and reveal optimal conditions. Remarkably, the actuation process is rapid, highly reversible, and maintains excellent performance over repeated cycles. These liquid crystal fiber arrays provide a safe contact with humans or other objects, making them highly suitable for applications in smart wearable devices and immersive interfaces.

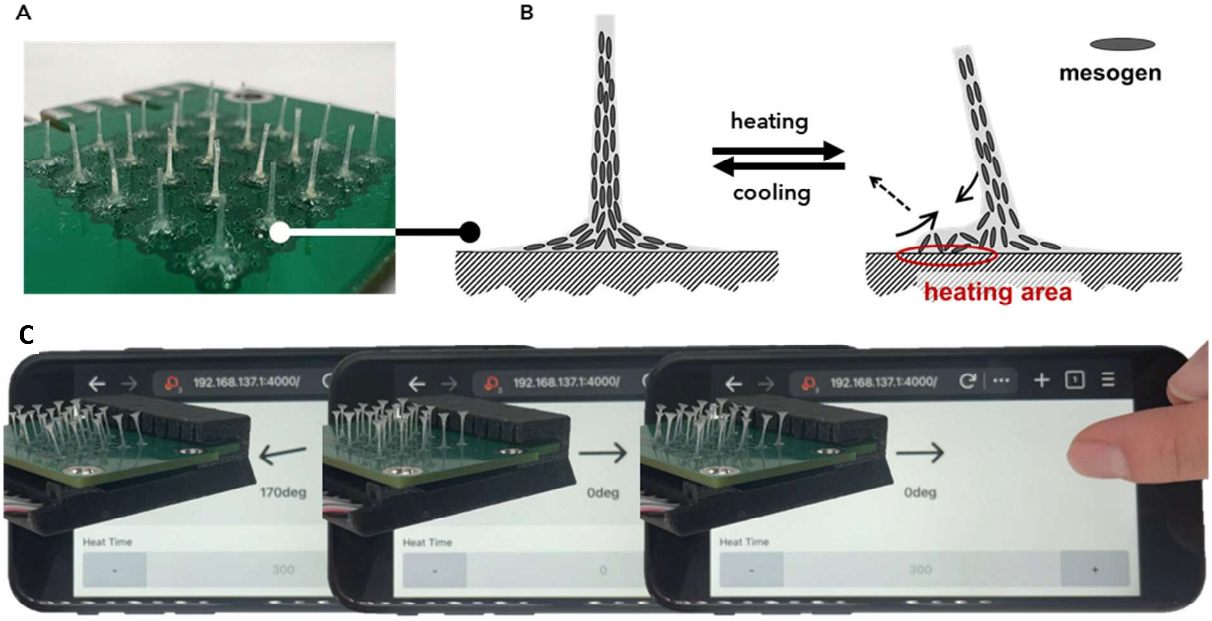

Figure 1: **A)** Liquid crystal fiber array. **B)** Schematic mesogen alignment and fiber actuation mechanism. **C)** Center: fibers at rest. Left and right: fibers directed by smartphone swipes.

Leveraging Low-Intensity Light for Omnidirectional Self-Oscillator with Scalability Potential

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Keywords: (Liquid Crustal Elastomer, Light-powered, Self-oscillation)

Self-oscillators driven by light and based on stimuli-responsive soft materials have garnered significant attention due to their potential in a wide range of robotic functions, including adaptation, autonomous locomotion, and energy conversion. However, the scalability and implementation challenges arising from the high energy density and unidirectionality of the excitation light beam have hindered their application. Here, we introduce a self-oscillator model employing a lampshade-like smart material assembly that responds to light stimuli. This assembly leverages a low-phase transition temperature liquid crystal elastomer as the photomechanical component (Figure 1a) [1], enabling twisting movements when exposed to low-intensity and incoherent light (Figure 1b). By incorporating a lampshade frame composed of four spiral segments, an innovative negative feedback mechanism is achieved, with an equal amount of light being shadowed to sustain oscillation under a constant light field from omnidirectional excitation (0º – 360º azimuth and 20º – 90º zenith) (Figure 1c). To showcase the concept's versatility, we fabricated oscillators of different sizes with diameters ranging from 6 mm to 50 mm, demonstrating the potential for scalable implementation [2]. This research offers new insights into the rapidly evolving soft material-based micro movements field.

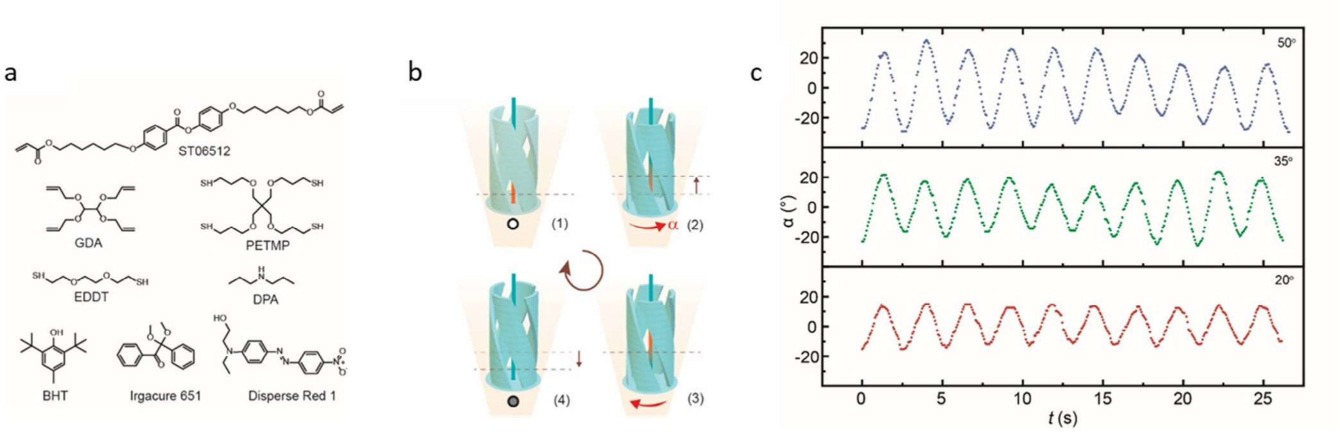

Figure 1. (a) Compounds used for fabricating the light-responsive LCE. (b) The self-shadowing mechanism for the self-oscillation through lampshade rotation. (c) Oscillation at different zenith angles.

Acknowledgments: Marie Sklodowska-Curie Grant Agreement 956150 (STORM-BOTS)

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Wee

Multimodal and Multistimuli 4D-Printed Magnetic Composite Liquid Crystal Elastomer Actuators

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Keywords: Liquid crystalline elastomer, 4D printing, magnetic soft robots, multi-modal devices, multi-stimuli actuators

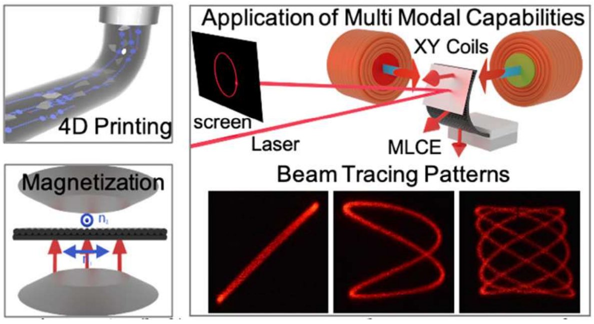

Figure 1: *(left) 4D printing and magnetization of printed MLCE elements (right) Multistimuli beam steering device*

Soft robotics applications usually demand fast and precise motion of compliant materials, such as magnetic elastomers (**ME**). These composites are usually created using silicone-based elastomers that entrap magnetic particles, allowing rapid motion of the actuators when subjected to external magnetic fields, still, they are not capable of exerting large forces or being programmed in their deformations with ease. In contrast to ME, liquid crystal elastomers (**LCE**) are being studied for their significant shape-changing capabilities, along with their high work capacity, when exposed to heat or light. These properties have made them ideal for developing soft robotic applications. Nevertheless, their relatively slow response compared to soft magnetic materials limits their application possibilities. Integration of magnetic responsiveness with LCEs has been previously attempted [1]; however, the LCE response is typically jeopardized at high volumes of magnetic microparticles (**MMPs**). Here[**1**] a multi-stimuli, magnetically active LCE (**MLCE**), capable of producing programmable and multi-modal actuation is presented. The MLCE, composed of MMPs within an LCE matrix, is generated through extrusion-based 4D printing (Figure 1, left) that enables digital control of mesogen orientation even at 1:1 (LCE:MMPs) weight ratio, a challenging task to accomplish with other methods. The printed actuators can produce significant mechanical forces when thermally actuated, as well as exhibit fast response to magnetic fields. When combining thermal and magnetic stimuli, modes of actuation inaccessible with only one input, are achieved. For instance, the actuator is reconfigured into various states using the heat-mediated LCE response, followed by subsequent magnetic addressing. The multi-stimuli capabilities of the MLCE composite expand its applicability where common LCE actuators face limitations in speed and precision. To illustrate, a beam-steering device developed using these materials is presented (Figure 1, right)

Acknowledgements: This work has received funding from the European Union's Horizon 2020 under the Marie Skłodowska-Curie grant agreement No. 956150 – STORM-BOTS

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D4

Augmented reality/virtual reality (AR/VR)

Advanced Guest-Host Liquid Crystal Devices: From Hollywood to Augmented Reality.

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Keywords: Augmented Reality, Guest-Host Liquid Crystals, Eyewear, ND Filters,

Guest-Host Liquid Crystals (GHLCs) have long been recognized for their unique property of controlling rapidly changing environmental lighting conditions. The anisotropic absorptive nature of dichoric dyes combined with the fast response of liquid crystals makes them suitable for advanced applications that require variable transmission, low power consumption, color neutrality, and rapid switching speeds. This work reviews novel and emerging uses of GHLCs, showcasing their versatility in diverse fields, pushing the boundaries of their utility. We will review a new groundbreaking liquid-crystal neutral-density filter used in the film industry that can be dynamically adjusted from ND0.3 to ND1.8 (Figure 1, left), offering 6-stops in a single device and allowing new cinematographic effects not possible otherwise. We will also show our progress developing a unique variable gradient GHLC filter.

Figure 1: Panavision LCND (left image), Snapchat AR Spectacles (right image).

Augmented Reality is another field having incorporated our GHLCs devices as part of a few core enabling technologies (Figure 1, right). Working in tandem with planar waveguides, display brightness does not get compromised due to high intensity ambient ilumination. We will also explore a new class of photodichroic materials promising to bring the next generation of Augmented Reality materials by combining absorptive dichroism with photochromism in a single device. The operation principles, manufacturing processes and future challenges of these advanced GHLCs applications will be discussed in detail.

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Plane parallel plates via nematic liquid crystal in optical imaging systems

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Keywords: LC devices, plane-parallel plate, varifocal devices, augmented reality

The light propagating in optical medium is related to the energy flow of electromagnetic wave corresponding to the Poynting vector. The direction of Poynting vector is parallel to the direction of the group velocity [1] and the direction of phase velocity is parallel to the direction of the wave vector. In the isotropic medium, there is no difference between the directions of Poynting vector and of wave vector, but not in anisotropic medium due to the dispersion relation [2]. When a light ray goes from an isotropic medium (usually air) to an anisotropic medium, Poynting vector and the wave vector split to each other depending on tilt angle of optical axis. The refraction angle of Poynting vector even turns out "negative" even the medium is right-hand material under certain conditions [2-4]. Plane parallel plates via nematic liquid crystals appears an anisotropic longitudinal shift. According to this feature, we adopt the plane parallel plate filled with horizontally aligned positive liquid crystal, so called the homogeneous LC plate, in augmented-reality system to alter the position of image by applying different operating voltage on the LC plate [5]. In this paper, the "negative refraction" in LC plane parallel plate is investigated based on Poynting vector theoretically. The effect of the negative refraction enables us to even enlarge the tunable range of the position of the virtual image in augmented reality. The impact of this study is to provide a varifocal LC devices for augmented reality and optical imaging systems.

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D5

Functional plasmonic nanostructures

Order and disorder induced by smectic liquid crystal topological defects on gold nanoparticles networks

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Keywords: smectic, topological defects, self-assembly, gold nanorods, plasmonic resonance

When it comes to composites of liquid crystals (LC) and nanoparticles (NP), topological defects become extremely interesting. Depositing a thin 8CB film on a rubbed PVA surface we observe a pattern of flattened hemicylinders of smectic layers, presenting linear topological defects together with a 2D melted grain boundary oriented along the direction of hemicylinders. Previous results from our group show that these defects are able to trap nanoparticles and to transmit them their geometrical shape, allowing the coexistence of different kinds of oriented nanoparticle assemblies [1]. We are currently interested in using gold nanoparticles, such as nanorods and very small nanospheres, that provide the composite with plasmonic properties. The nanospheres we use have a diameter of less than 3nm, which is comparable with the smectic layers period. This characteristic makes them interact differently with the LC with respect to bigger NPs [1]. Combining X-Ray diffraction, optical spectroscopy and simulations we reveal that anisotropic light absorption is induced by the coexistence of 2D hexagonal NP arrays in the 2D grain boundaries and 3D NP networks commensurate to the smectic layers outside the defects (Fig. 1). When using nanorods coated with thiol-terminated polystyrene, we create different NP assemblies: optical spectroscopy controlled by light polarization with respect to the smectic hemicylinders direction (Fig. 2) show that only the defects are filled by the nanorods: chains are formed with a tip-to-tip configuration at small concentration, coexisting with ribbons at large concentration. In the ribbons, nanorods are side-to-side and perpendicular to the chains. This latter orientation is perpendicular to the one obtained with nanorods functionalized with alkyl chains [2]. This suggests that the ligands play a fundamental role in the interaction between the nanoparticles and the liquid crystal. These results show that playing with ligands' nature will lead us to control the NP organization, in particular a control of the nanorod orientation and therefore of the anisotropic light absorption.

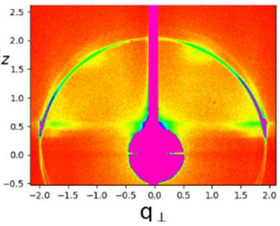

Figure 1. GISAXS pattern of hemicylinders containing small gold nanospheres organized in tridimensional networks.

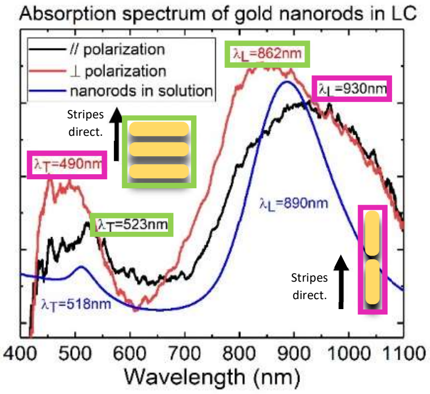

Figure 2. Absorption of gold NR in LC.

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D7

Conductive liquid crystals

Donor and Acceptor binary mixtures of phthalocyanine mesogens and C_{60} derivatives: miscibility, mesomorphism and carrier mobility

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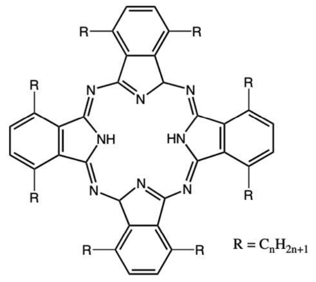
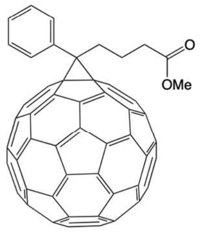
Keywords: liquid crystal, organic semiconductor, phthalocyanine, C_{60}

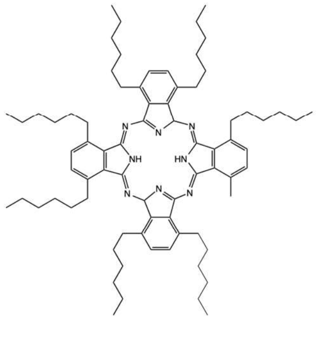
Composite materials based on liquid crystals have been studied so extensively as to polymer systems. However, low-molecular weight systems are also interesting as to self-construction of molecular-scale structure. Especially, this is an important issue for the application to electronic materials and devices such as organic photovoltaics. Once, the binary systems of non-peripherally substituted phthalocyanine mesogen (**C6PcH$_2$**) and a C60 derivative (PCBM) was reported to show a certain efficiency for photo-electronic conversion [1] and the mixtures were studied as organic photovoltaic system which performed up to 5% of photoconversion efficiency [2]. In this mixture, the enhanced mobility was observed for a component ratio [3]. In this work, miscibility of PCBM for the mesophase of **CnPcH$_2$** (n=5, 6, 7 and 10) and the carrier mobility behaviour were investigated.

The mixtures of **CnPcH$_2$** and PCBM show that the miscibility of PCBM into the Col mesophase depends on alkyl chain length. The elongation of chains leads to depression of the miscibility, though the phase separation takes place when the component ratio of PCBM is 5 ~ 25 mol%. The enhanced miscibility was not observed for **Me5C6PcH$_2$** of which one hexyl chain is replaced by a methyl group to make a space for PCBM positioning. The charged carrier mobility of those systems was evaluated by TOF(Time-Of-Flight) technique, which would relate to morphological structures of the systems. The temperature dependent nature of mobility gets noticeable in the mixtures for Col mesphases, indicating thermally enhanced disordering is more effectively caused.



CnPcH$_2$





Me5C6PcH$_2$

Acknowledgements: This work was supported in part by JSPS ALCA Program, Grant Number 15H03552,18H04514.

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Improvement of solubility for liquid crystalline materials by chemical modification in the end of side chain and their organic transistor characteristics

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Keywords: Smectic E phase, Ph-BTBT, high solubility, mobility

Mono-alkyl phenyl-benzothienobenzothiophene (Ph-BTBT) derivatives, which exhibit a highly ordered liquid crystal phase, smectic E (SmE) phase, give us uniform and molecularly flat polycrystalline thin films by solution process, when they are fabricated by using a SmE thin film as a precursor for a crystalline thin film. Organic field effect transistors (OFETs) fabricated with the uniform films show mobility over 5 cm^2/Vs in spite of polycrystalline thin films [1]. However, there are remaining issues of a low solubility, for example, 2g/L for decyl Ph-BTBT (Ph-BTBT-10) in toluene at room temperature. In this presentation, we have synthesized new Ph-BTBT derivatives chemically modified with an ether group in the end of side chain, Ph-BTBT-(CH$_2$)n-O-CH$_3$: Ph-BTBT-nO-1, where n is the number of carbon atom attached to BTBT-core, and evaluated liquid crystallinity, solubility, film morphology, and FET characteristics. Ph-BTBT-nO-1 derivatives show SmE phase and have higher solubility for polar solvent such as anisole compared with the solubility of Ph-BTBT-n for non-polar solvent such as toluene. The solubility of Ph-BTBTnO-1 derivatives is 3 – 12 g/L in anisole, which decreases as n is increased. Crystalline thin films were fabricated by spin-coating at SmE phase and the resulting thin film was very flat and uniform. We have fabricated the bottom-gate bottom-contact type OFETs with the uniform polycrystalline thin films of Ph-BTBT derivatives. OFETs showed excellent p-channel operation and FET mobility was increased when as-fabricated FETs were thermally annealed. The FET mobility showed 6.5 cm^2/Vs in Ph-BTBT-12O-1 as shown in Fig. 1. We conclude that chemical modification in the end of side chain with an ether group is an excellent method to increase the solubility for polar solvents, while keeping the high mobility.

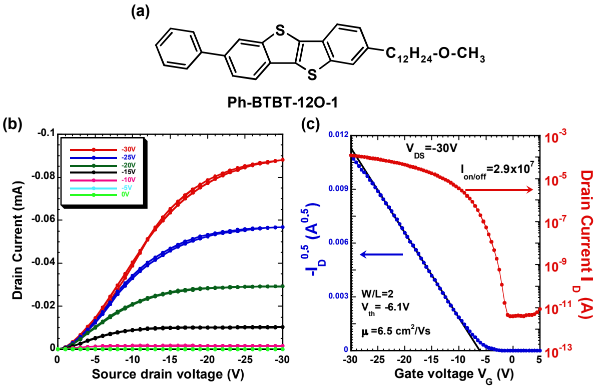

Figure.1 Ph-BTBT-12O-1 FET characteristics. (a) Chemical structure, (b) output, (c) and transfer characteristics in saturation regions.

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D8

Liquid crystal lasers and nonlinear optical devices

An integrated electromagnetic, molecular and lasing model for liquid crystal laser optimization

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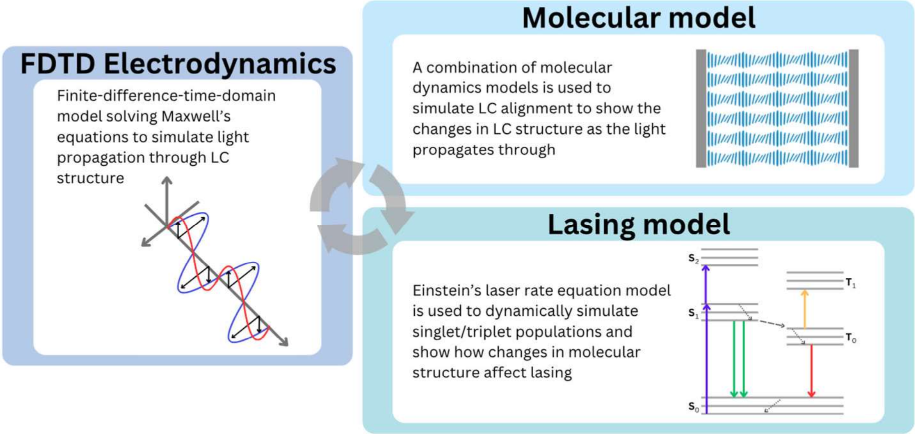
Keywords: Liquid crystal lasers, FDTD, molecular dynamics

Dye-doped chiral nematic liquid crystals have self-organizing optical cavities enabling low cost, micro-scale photonic band-edge lasers, with a broad wavelength tuneability throughout the visible spectrum [1]. Liquid crystal (LC) lasers have prospective applications in imaging and sensing where a precise and customizable wavelength is required [2]. However, factors such as output stability, maximum average power and repetition rate, currently limit laser performance and possible commercialization. Some of these detrimental effects are temporary and reversible in nature (fatigue mechanisms), such as thermal build-up, triplet state excitation, or optically-induced reorientation from the pump laser [1]. Other effects may be more permanent, such as photobleaching of the dye at extreme input powers [1]. However detailed analysis and quantification of these different effects has not been thoroughly investigated.

We present the latest update on a comprehensive LC laser simulation, comprising of three linked models (Figure 1), to investigate the above phenomena. Pump propagation through the LC is simulated using FDTD method solving Maxwell's equations. Landau-de Gennes free energy minimization (including Beris-Edward model) is used to simulate LC alignment [3]. Finally, lasing output is predicted using rate equations. This approach will provide better understanding of the relative contributions of fatigue mechanisms in LC lasers, enabling optimization of device architecture and pump parameters to maximize laser stability and output power.



FDTD Electrodynamics

Finite-difference-time-domain model solving Maxwell's equations to simulate light propagation through LC structure

Molecular model

A combination of molecular dynamics models is used to simulate LC alignment to show the changes in LC structure as the light propagates through

Lasing model

Einstein's laser rate equation model is used to dynamically simulate singlet/triplet populations and show how changes in molecular structure affect lasing

Figure 1: Schematic representation of liquid crystal laser model

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Coherent Up-Conversion in a Polar Liquid Crystal via Simultaneous Intra-Cavity Lasing and Frequency Doubling

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Keywords: Laser, Second Harmonic Generation, Nonlinear Optics, Wavelength Conversion, Ferroelectrics

Photon up-conversion is a process that harvests higher energy photons from lower energy photons. There have been proposed and demonstrated many types of photon up-conversion via various physico-chemical optical processes, but most of those are incoherent and not so useful for photonics applications especially those utilizing phase detection technique. However, in some nonlinear optical processes, one may obtain coherent up-converted photons - The simplest coherent photon up-conversion process is the optical second harmonic generation (SHG), which is an instantaneous frequency doubling process converting two photons to one photon with coherency. Another slightly more complicated example of photon up-conversion via the nonlinear optics is the optical parametric generation, which is tunable photon conversion process and thus more useful, but this requires complicated optical setup to achieve phase matching and high power input for stimulation. In this study, we demonstrate an easy and simple technique to achieve coherent photon up-conversion using a recently-found polar nematic liquid crystal (PNLC) [1, 2]. PNLC was doped with an infrared laser dye providing laser gain. The used liquid crystal cell was conventional sandwich-type but with dielectric high reflectors so that it also worked as a Fabry-Perot etalon. Since PNLC is a non-centrosymmetric optical medium and thus inherently activated for even-order nonlinear optics, this makes it possible to up-convert infrared photons into ultra-violet ones with coherency, via the simultaneous coherent processes of lasing and frequency doubling. With the aid of liquid crystallinity, the output up-converted light intensity can be modulated by external stimuli such as electric field application or temperature variation. Realization of such an unconventional optical function may lead to various unique ideas of applications of PNLCs.

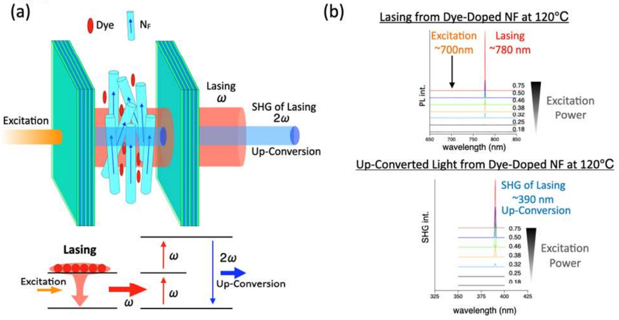

Figure 1: Our intra-cavity coherent up-conversion process demonstrated in this study.

Acknowledgements: The authors acknowledge JSPS KAKENHI, JST SICORP and JST CREST for financial support.

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Microfluidic laser based on polymeric chiral nematic liquid crystal cavity

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Keywords: lasers, microfluidics, liquid crystals, chiral materials, polymers

The fascinating benefits of liquid crystal-based lasers, such as ease of fabrication, miniature size, high compatibility with various containers, tunable wavelength, controllable polarization, and so on, make liquid crystal-based lasers highly potential for imaging applications, such as light sources for biomedical microscopy and holographic images [2,3]. However, liquid crystal-based lasers can last emitting only for a short time, around seconds to tens of seconds, because of the thermal fluctuation of the liquid crystal laser cavity and photo-bleaching of the fluorescence dye.

In this work, we propose the first miniature dye laser integrating a microfluidic gain medium and a self-organized laser cavity composed of a chiral nematic liquid crystal polymer template, as shown in Fig. 1(a). By continuously infiltrating fluidic gain medium into the chiral nematic polymer template, the lasting time for the lasing emission can be significantly prolonged compared to the static one, as shown in Fig. 1(b) and 1(c). The prototype proposed in this work moves liquid crystal lasers further toward practical applications.

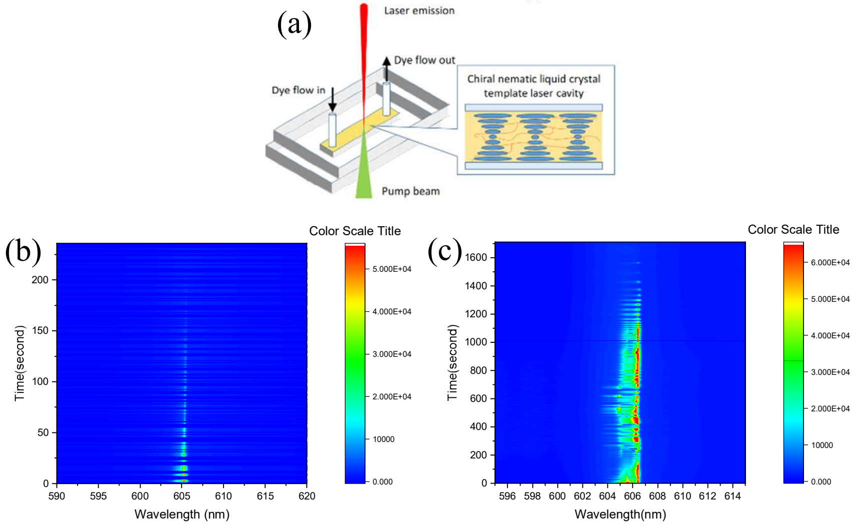

Figure 1: (a) Schematics for the microfluidic laser, and the evolution of the emission spectra when the fluidic is (b) static and (c) with the the flow rate of 5 µl/min.

Acknowledgements: The authors would like to express the utmost gratitude to NSTC of Taiwan for financially supporting this research under the project number NSTC 109-2112-M-259-009-MY3 and NSTC 112-2112-M-259-011.

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Nonlinear and thermo-optical properties of liquid crystals doped with carbon quantum dots

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Keywords: Thermal effects, Nonlinear optics, Photodegradation, Field-induced reorientation

The phenomenology of nonlinear optical response in soft materials is a long-standing issue, widely investigated due to their potential application in optoelectronic devices. In this context, the thermal and nonlinear optical properties of a cyanobiphenyl liquid crystal are investigated, considering the addition of carbon dots synthesized from different conjugated dyes. The generation of local disorder and the photostability of doped liquid crystal samples are analyzed, determining the changes in the transition temperatures associated with the photoexcitation of guest nanoparticles. Using the time-resolved z-scan technique in photostable samples, the nonlinear optical response of planar nematic cells is investigated in the excitation regime below the optical Freedericksz threshold. Z-scan measurements reveal that adding carbon dots increases the nematic host's nonlinear refractive contribution, being related to thermally induced changes in the extraordinary and ordinary refractive indices. In particular, adding carbon dots enhances the absorption coefficient of liquid crystal at the laser wavelength, thus increasing the heat generation in the sample upon photoexcitation. The effects of carbon dots are less pronounced when an external electric field is applied, reorienting the nematic director. The present findings reveal that the addition of carbon dots can be used to appropriately modify the nonlinear optical properties of liquid crystal matrices, thus making such hybrid soft materials promising candidates for optical devices. Liquid crystals doped with carbon dots can be exploited to obtain tunable optical metadevices based on a thermal variation of nematic birefringence, including metalenses, dynamic beam deflectors, and active all-dielectric metasurfaces.

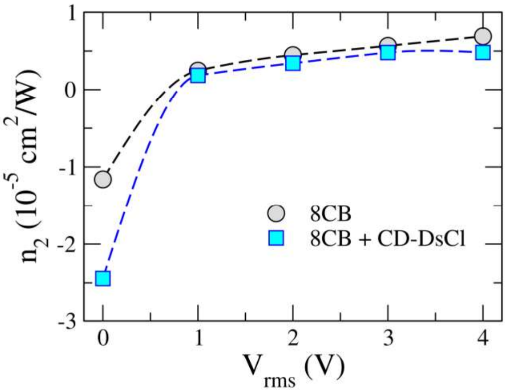

Figure 1: Nonlinear refractive index of pristine (gray circles) and doped (blue squares) 8CB samples as a function of an external applied voltage

Acknowledgements: CNPq INCT-Fcx (CNPq – 465259/2014-6), FAPEAL (E:60030.0000002288/2022)

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Photonic eigenmodes of 2D cylindrical cholesteric liquid crystal resonators

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Keywords: cholesteric liquid crystal, laser, photonic eigenmode, resonator, Q-factor

Cholesteric liquid crystals (CLCs) exhibit a periodic helical structure that partially reflects light with wavelengths comparable to the period of the structure, thus performing as a one-dimensional photonic crystals. Lasing from flat CLC cells has been well researched in the past [1]. Recently, we have shown that the characteristics of 1D CLC lasers are connected to the eigenmodes of the self assembled CLC lasing cavity [2]. Lasing from other cholesteric structures, like CLC droplets has also been reported in the past [3], but has been less researched theoretically and numerically. In this work we numerically calculate photonic eigenmodes in a 2D cylindrical cholesteric liquid crystal resonator with the helical axis pointing in the radial direction (shown in Fig. 1a). Such lasing cavity mimics the director profile in selected cross sections of 3D CLC droplets. We show that the spectrum (Fig. 1b) of the resonator consists of different types of photonic modes, like band edge modes (Fig. 1c), whispering gallery modes and defect modes. We characterize the modes in terms of Q-factors and analyze their dependence and dependence of the spectra on different parameters, like radius, pitch size, refractive indices etc. Finally, we calculate the eigenmodes and the spectrum of the spiral CLC structure, another characteristic cross section of a 3D CLC droplet [4]. Overall the work is a step towards better understanding of optical properties of 3D CLC droplets and CLC structures in general.

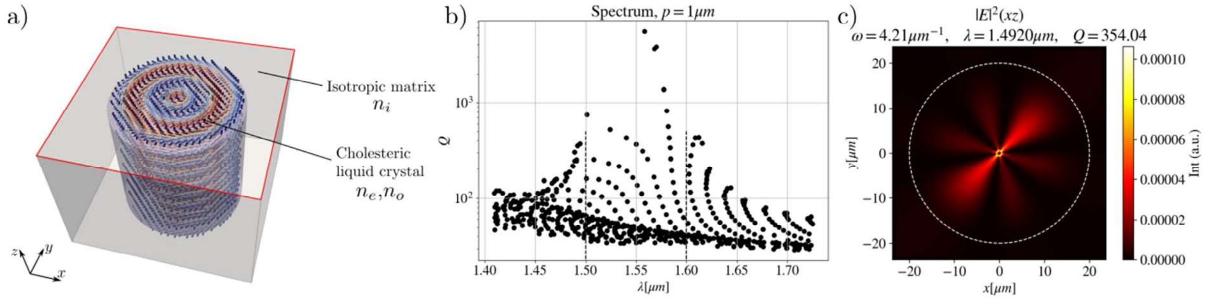

Figure 1: a) 2D cylindrical CLC resonator. b) Calculated spectrum of photonic eigenmodes. c) Intensity profile of a selected band edge mode.

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Photonic modes and lasing properties in different cholesteric liquid crystal structures

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[2]Jožef Stefan Institute, Ljubljana, Slovenia

Keywords: cholesteric liquid crystal, photonic crystal, resonator, laser, quality factor

Cholesteric liquid crystals (CLCs) with a periodic helical structure act as photonic crystals and thus partially reflect light with wavelengths comparable to the period of the structure. Possessing these properties, CLCs can be utilized as optical resonators or even as micro-lasers if doped with organic dye [1,2]. We present the findings of numerical studies based on finite-difference time-domain (FDTD) and finite-difference frequency-domain (FDFD) methods of light transmission [3], amplification and lasing in different CLC structures with gain material. These optical phenomena were studied not only in simple planar cells but also in cylindrical and spherical structures. We show numerically calculated electric field profiles of photonic eigenmodes, their quality factors, and corresponding lasing thresholds. Overall, this presentation summarizes the optical properties of CLC resonators that could be important for the design of liquid crystal micro-lasers and other soft-matter-based photonic devices.

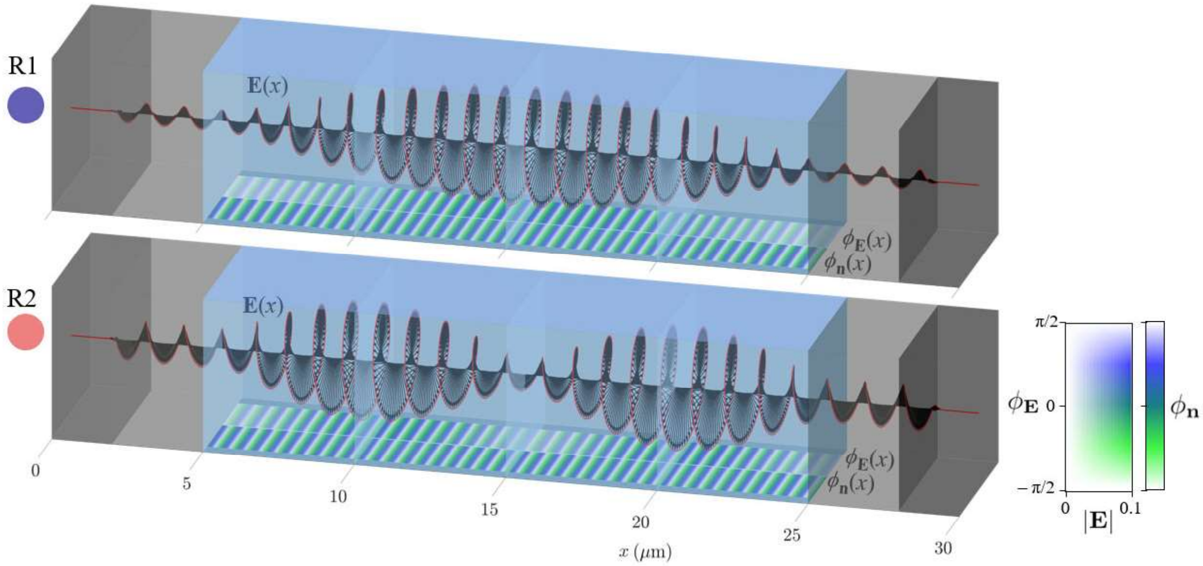

Figure 1: Electric field profiles of band-edge modes in 1D planar cholesteric liquid crystal cell. Colours at the bottom surface show the orientation of electric and director field. [3]

Acknowledgements: Funding from the European Research Council under the European Union’s Horizon 2020 Research and Innovation Program (Grant Agr. No. 884928-LOGOS).

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Quantum optics with liquid crystals: tunable generation of entangled photons from ferroelectric nematics

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Keywords: entangled photons, photon pairs, quantum optics, spontaneous parametric down-conversion, ferroelectric nematic liquid crystal.

Quantum light sources are devices that generate light with distinct quantum features, most frequently single-photons or photon pairs, and are essential in various applications such as quantum communication, quantum computing, and quantum metrology. The most common way of generating (entangled) photon pairs is spontaneous parametric down-conversion (SPDC) where a nonlinear crystal (e.g. lithium niobate (LN), beta barium borate (BBO), etc.) is used to split a single incoming photon into two photons. In the last several decades there were no revolutionary advances made regarding these nonlinear materials. In fact, LN is still one of the best and one of the most used nonlinear crystals for the generation of photon pairs more than 50 years after it was used for the first demonstration of SPDC. Further, current sources lack tunability and are designed for the generation of a particular quantum state.

Recently, ferroelectric nematic liquid crystals (FNLCs) have been discovered, which have polar ordering, leading to a large dielectric constant, a strong response to an electric field, and a very high optical nonlinear response. Among other possible uses, FNLCs have strong potential for applications in tunable nonlinear devices. A strong second harmonic generation (SHG) has been demonstrated in FNLCs, but they have never before been employed for generating photon pairs.

Here, we demonstrate for the first time the generation of entangled photons from a FNLC [1]. This is also the first demonstration of SPDC in any organic material. The conversion efficiency is on par with the best nonlinear crystals available today, with the added benefit of tailoring and tuning the output of the source. We show that by simply adjusting the twist of the molecular orientation along the sample, almost any polarization state can be generated, including states with maximum entanglement. Additionally, by applying only a few volts, we can drastically alter both the emission rate as well as the generated state of photon pairs which enables real time tunability. This is the first source of photon pairs which offers such tunability.

The rich self-assembled and topological structures in LC could in future enable sources, which emit tunable complex structured quantum light.

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Random light in strongly disturbed liquid crystals

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Keywords: light scattering, liquid crystal, cholesterics, photonic band gap, random medium

Multiple scattering of light in strongly disordered optical media helps waves to revisit a previously irradiated unit of volume providing essential feedback for lasing, manifested by narrow spikes atop the regular fluorescence spectrum. Random lasing (RL) has been observed in a wide range of materials and scattering regimes [1] being quite prospective from the application standpoint as well as for fundamental studies.

Contrary to the conventional RL media characterized by a very high refractive index of scatterers, the phase contrast in liquid crystalline (LC) media is usually quite small. With regular LC domains being of the order of several to tens of microns the van de Hulst approximation becomes valid comprising large, optically soft spheres with low efficiency coefficient $Q \ll 1$.

Chiral nematic liquid crystals (CLC) with a self-assembled supramolecular helical structure constitute a natural photonic crystal revealing a photonic bandgap (PBG) visible as the selective reflection of light (SR). Optical properties of CLC and, hence, the character of light propagation varies drastically within the range of wavelengths in the proximity of PBG.

A supramolecular helical structure of chiral nematic liquid crystals (CLC) makes these a natural photonic crystal that is self-assembled at the nano-scale material revealing a photonic bandgap (PBG) that appears as selective reflection of light (SR). Periodicity of the helix and, hence, the spectral position of the SR is easily adjustable in CLC within an extremely wide range in different ways. Optical properties of CLC and, hence, the character of light propagation vary drastically within the light wavelength range in the proximity of PBG. The existence of SR greatly increases scattering differential cross-section that results in a substantial enlargement of the transport mean free pass, consequently, lowering the lasing threshold in CLC [2].

We present a model for numerical simulations of light propagation in an arbitrary system of randomly distributed scattering units accounting for multiple light scattering in the geometry optics approximation. Applied for strongly disturbed LC-based media the model allows for distinguishing the presence of the CLC selective reflection due to the evident changes in the light diffusion diagram.

The calculations also confirm the increase of the path length or dwell time of light inside the gain medium accompanied by non-resonant localization of light that could greatly facilitate optical amplification corresponding well to the experimental data. Further adjustment and verification of model parameters via detailed comparison with experimental data is foreseen.

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When structured light meets liquid crystals

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Keywords: liquid crystals; structured light; spherulites; self-assembly

Structured light plays an important role in modern optical technologies such as high-capacity communication and particle manipulation. The highly ordered donor-recipient columnar stack is composed of alternating disc-shaped aromatic molecules, which is self-assembled by an electron-rich donor and an electron-deficient acceptor. The proposed strategy provides promising and wide opportunities in easy generating broad band vector optical vortices at optical frequency for advanced applications, especially in polychromatic optical vortices multiplexing field.

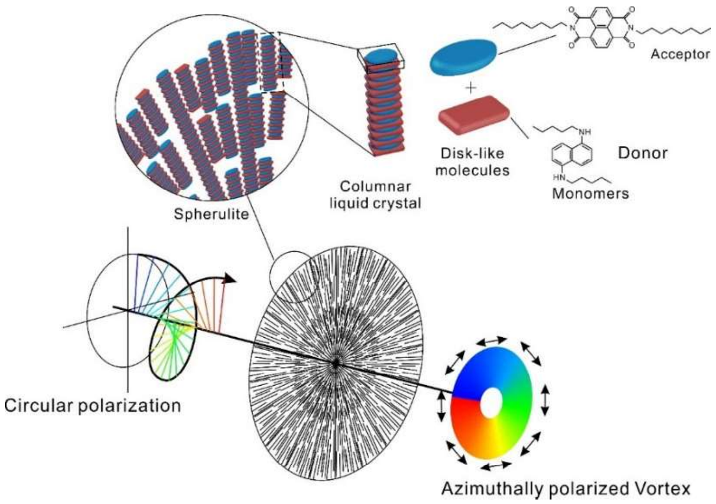

Figure 1: Schematic representation of the spherulite material and the generation of the optical vortex with azimuthal polarization.

Acknowledgements: This work was supported by the following grants: National Key R&D Program of China (Grant No. 2022YFB3806000), National Natural Science Foundation of China (Grant No. 11974203), The Basic Science Center Project of NSFC (Grant No. 52388201), Basic Science Centre Program of Natural Science Foundation of China (NSFC) (Grant No. 52388201), National Key R&D Program of China (Grant No. 2022YFB3803500), the NSFC (Grant No. 52027817).

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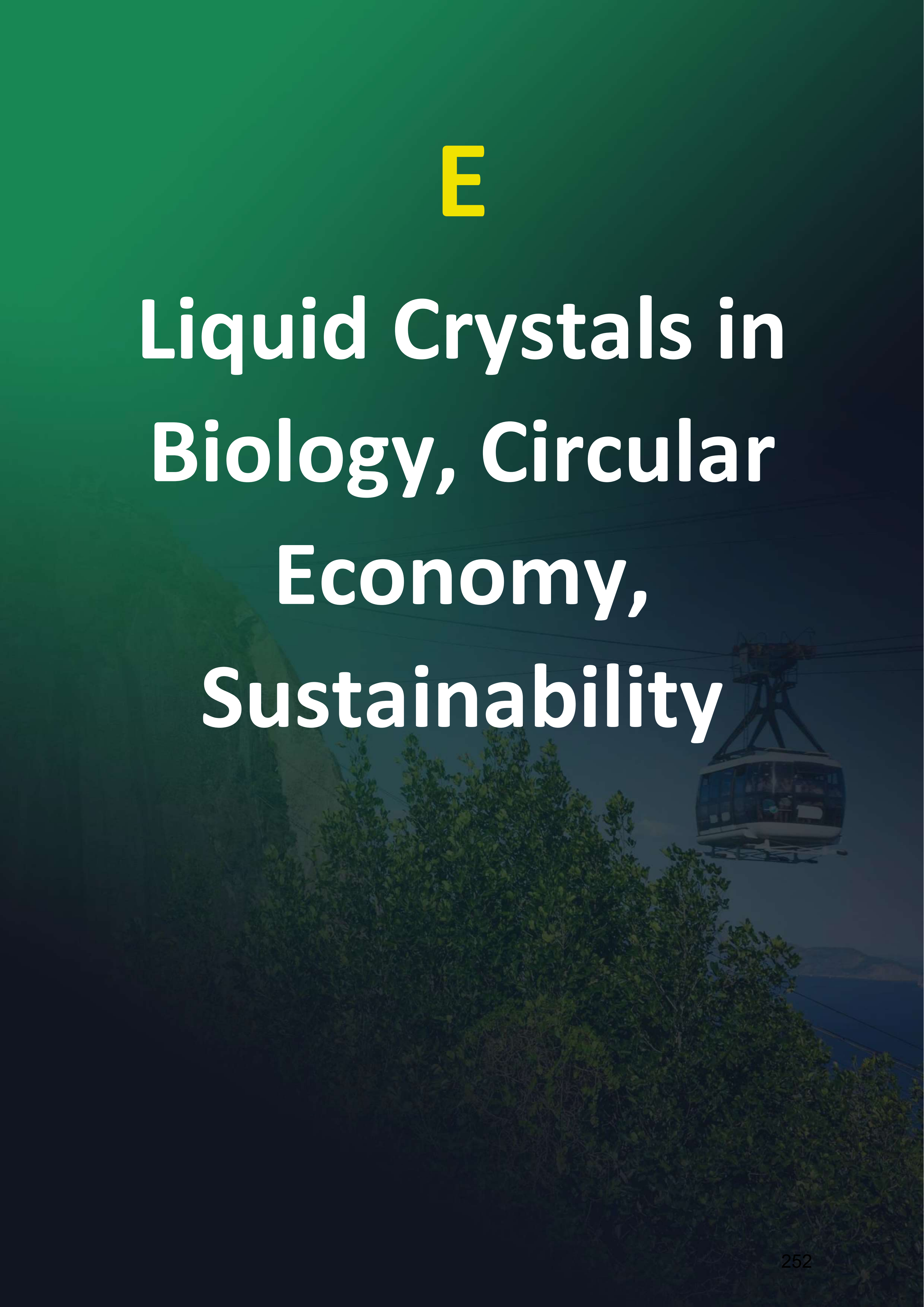

E

Liquid Crystals in Biology, Circular Economy, Sustainability

E1

Smart textiles, energy and environmental issues, sustainability, etc

DCM Alternatives for use in Steglich Esterifications, for Green and Sustainable Liquid Crystal Syntheses

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Keywords: Organic Synthesis, Sustainability, Green Chemistry, Ferroelectric Nematic

The Montreal Protocol (1989) banned carbon tetrachloride as a solvent due to its ozone depleting properties and was largely replaced by dichloromethane (DCM). [1] Halogenated solvents must now be phased out. DCM is hepatotoxic, neurotoxic, carcinogenic, and the cause of at least 85 deaths from 1980 through acute exposure. [2–5] Moreover, it has been shown to damage the ozone layer, [1,5] hence, the US EPA have proposed a ban. DCM needs to be urgently replaced with less hazardous solvents, according to the ACS Green Chemistry Institute Pharmaceutical Roundtable. [5]

We screened twenty green and sustainable solvents to find the most efficacious DCM alternative for the synthesis of a typical liquid crystal such as CZP-5-N, [6] (figure 1). Several factors are considered: yield, environmental factors, and health and safety concerns. The best performing solvent was then used in the synthesis of other common liquid crystal substrates, giving excellent results, even for electron poor phenols. Esters are highly prevalent in the new ferroelectric nematic phase, due to their role in polar conjugation, making sustainability in this space crucial for the next generation of liquid crystal materials.

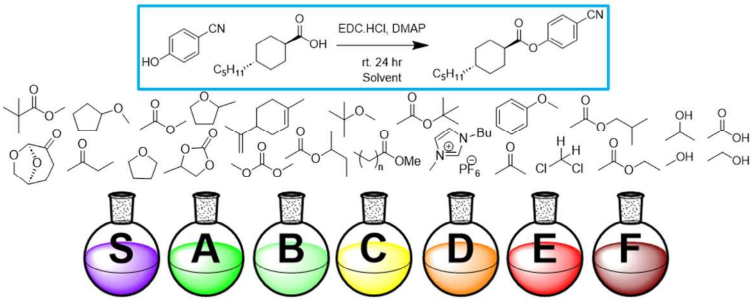

Figure 1: Solvents considered for the synthesis of CZP-5-N in this systematic study as a replacement for DCM in Steglich esterification reactions.

Acknowledgements: The authors thank the SOFI^2 CDT for funding a PhD program for WO; RJM thanks UKRI for award of a Future Leaders Fellowship.

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E2

Self-assembly in nature, colloids and chromonics

Cellulose Nanorods liquid crystalline hierarchical cholesteric structures

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Keywords: Cellulose Nanorods, twisted structures, hierarchical cholesteric liquid crystals

Self-organized cellulose-based hierarchical twisted structures are all around us, mainly in plants, being a source of cellulose materials and a motivation to fabricate systems with properties that mimic natural designs, functions, and properties. At the genesis of some of these structures, for example, those found in the cell wall of some fruits and leaves, are cellulose nanocrystals (CNC) that can assemble in right and left-handed structures resembling cholesteric liquid crystalline phases [1- 4].

This presentation first addresses cellulose-based chiral molecular systems and nanoscale helicoidal arrangements. Attention is given to cellulose nanocrystals, water interactions, and hierarchical twisted cellulose liquid crystalline structures obtained from cellulose nanocrystals water-based suspensions. Special attention will be given to new results concerning phase and chirality inversion cellulosic systems.

Acknowledgments: This work was financed by national funds from FCT—Fundação para a Ciência e a Tecnologia, I.P., in the scope of the projects LA/P/0037/2020, UIDP/50025/2020 and UIDB/50025/2020 of the Associate Laboratory Institute of Nanostructures, Nanomodelling, and Nanofabrication—i3N. European Cooperation in Science & Technology (COST) Action European Topology Interdisciplinary Action (PhoBioS CA21159).

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Nematic alignment in cell monolayers guided by topography

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Keywords: active liquid crystals, topological defects, cells

Many recent studies have shown that the liquid crystalline organization of certain types of living cells affect their ability to communicate, their migration patterns and the mechanical properties of tissues. Moreover, topological defects in the cell alignment can change the expression of certain proteins, promote apoptosis and influence tissue morphogenesis [1]. Each of these phenomena is the result of a delicate interplay between biological, chemical and physical elements, which eventually determine the fate of the cells. Unlike other types of active liquid crystals, in fact, cells have active mechano-responses that are sensitive to chemical and physical cues.

In our research we impose and control distortions in monolayers of fibroblast cells using micro-patterned surfaces with varying shapes and chemistry. These constitutes useful platforms to characterize the alignment and the organization of the fibroblasts. We can impose topological defects in the cell alignment using patterned micro-ridges and characterize the influence of defects on cell density, alignment, shape and dynamics [2, 3]. We show that topological defects strongly affect the cells' density and shape, and further that this behavior is affected by the geometry of the ridges and by the strength of the adhesion. We can enhance or suppress collective behavior by modifying the geometry of the ridges and the cell-substrate adhesion. Finally, we confine the cells in wells with corners and wedges to characterize the cells' tendency to splay or bend near corners, to determine the elastic anisotropy of the monolayer.

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Acknowledgements: Novo Nordisk Foundation grant 21OC0065453

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Forces on a pair of parallel plates in an electrolyte solution: the effects of charge regulation

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Keywords: lyotropics, membranes, colloids, charge regulation

We consider an example from biology: vesicles with double membranes, which we model as a pair of parallel plates in an electrolyte solution or lyotropic liquid crystals in a lamellar phase. We picture the membrane walls or the lamellar sheets as colloidal plates. The charge of the colloidal particles (plates) immersed in an electrolyte solution is not constant: it depends on the pH and on the electrolyte concentration inside the suspension(1),(2). The process of charging the colloidal particles is denoted by charge regulation. We search for the repulsive force on each plate as charge regulation is achieved. The effective charge on the plates is obtained by integrating a Poisson-Boltzmann equation using a Runge-Kutta fourth-order algorithm combined with a Newton-Raphson root-find ing routine. The repulsive force on each plate at a given separation (gap) can be obtained using the Gouy-Chapman model of the diffuse layer and the additional electric stress local stress (in the case of plates carrying unequal charges). The dependence of the repulsive force on the gap width is obtained numerically. Of course the stability of the plates (vesicles) is guaranteed by equilibrating the electrostatic force on each plate and the surrounding suspension net hydrostatic force.

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Liquid crystalline structuring in photonic aqueous suspensions of high aspect ratio clay nanosheets

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Keywords: Clay colloids, non-iridescent structural colors, nematic and lamellar ordering

Aqueous suspensions of high-aspect ratio 2D clay nanosheets, have been investigated using Small Angle X-ray Scattering (SAXS). The high aspect ratio of synthetic fluorohectorite clays allows for investigation of liquid crystalline orientational order for relatively large nanosheets spacings, in a range which also can produce structural coloration. Various clay and salt concentrations were investigated. Particular attention is given to the confinement caused by container geometry, and thus cylindrical (capillary), flat (cuvette), and spherical (droplet) confinements were investigated. The SAXS data suggest coherent regions that have a nematic orientational distribution that is linked to the container geometry and suspension packing. For all geometries the analysis suggests that these coherent regions have a 1D lamellar periodic intra-structure with uniform nanosheet spacing determined by the clay concentration and a typical coherence length in the range of 200 to 500 nm.

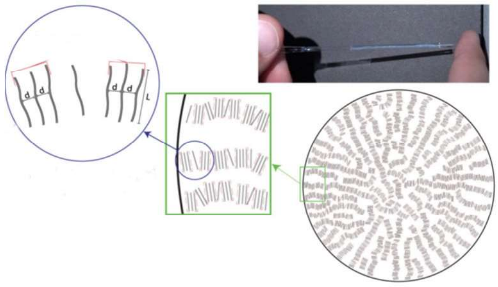

Figure 1: Aqueous photonic suspension of high aspect ratio clay nanosheets, in capillary confinement Image: Blue color in capillary. Sketch: SAXS interpretation of combined nematic and lamellar structuring.

Acknowledgements: Research Council of Norway, German Science Foundation, EU Horizon 2020

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Liquid crystal-promoted polymerization of RNA nucleotides

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Keywords: RNA, Self-Assembly, Lyotropic, Origin of Life

One prominent theory concerning the origins of life is the "RNA world" hypothesis, proposing that ribonucleic acid (RNA) was the first bio-macromolecule to emerge in the prebiotic world due to its combined ability to store genetic information and catalyze chemical reactions, including its own synthesis[1]. However, one of the primary concerns with this hypothesis is its lack of a highly efficient, prebiotically compatible mechanism capable of explaining the formation of RNA chains from simple nucleotides.

This study explores the reactivity and self-assembly abilities of prebiotically compatible[2] 2'-3' cyclic nucleosides monophosphates (cNMP) during drying at various pH levels. We observed, while drying at room temperature, the formation of liquid crystalline phases and birefringent aggregates in solutions of individual nucleotides and mixtures. When such samples are cyclically dried and rehydrated in basic environments, nucleotides spontaneously oligomerize with a reactivity peak around pH 10, resulting in condensation yields up to 70%. This behavior suggests an important templating role of liquid crystal and/or crystalline self-assembled structures in favoring their abiotic ligation.

This study, while strengthening the RNA world hypothesis, highlights the crucial role of nucleic acid self-assembly in promoting their own prebiotic appearance and convey the suggestion that prior to the RNA world there could have been a "Liquid Crystal World".

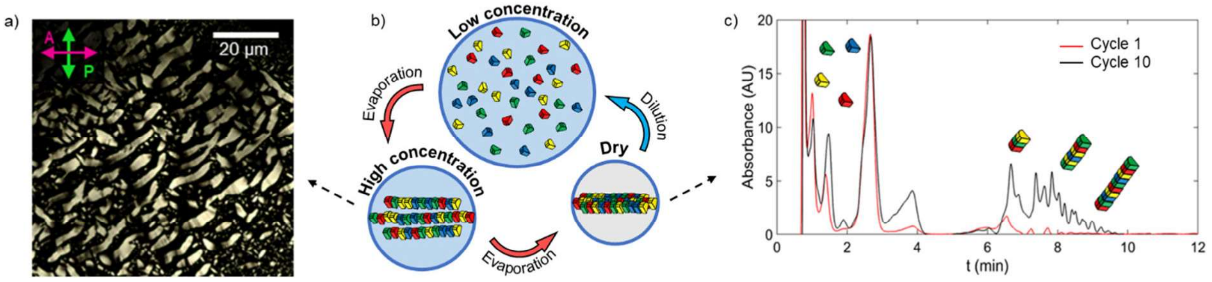

Figure 1: a) Polarized optical microscopy image of a concentrated sample of 2'-3' cNMPs at pH 10. b) Schematic representation of the wet-dry cycling. c) HPLC chromatograms showing the formation of RNA oligomers upon wet-dry cycling.

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Pumping and mixing active nematics with asymmetric inclusions

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Keywords: Active nematics, fluid dynamics, active matter, liquid crystals.

Active nematics are formed by self-propelled elongated particles that tend to align with their neighbours. Examples are swarming densely packed bacteria and microtubule-kinesin-mixtures. Unconfined active nematics often become turbulent with topological defects following chaotic trajectories. In this work, we use lattice Boltzmann simulations and experiments with microtubule-kinesin mixtures to investigate the control of active turbulence using axisymmetric solid obstacles like triangles. We find that if the obstacles have the correct dimensions, they will induce directed flow which could be used as a two-dimensional microfluidic pump. Because there are also flows in the perpendicular direction, a lattice of triangles also provides efficient and directed mixing in active nematics.

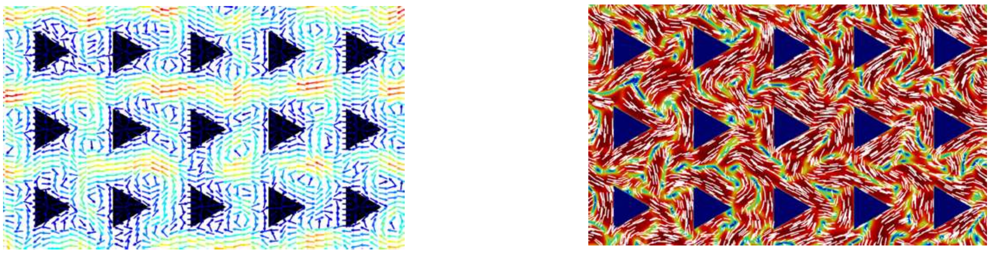

Figure 1: Velocity and director field of the active nematics guided by the solid triangles.

Acknowledgements: This work was funded by the Portuguese Foundation for Science and Technology (FCT) under the contracts: PTDC/FIS-MAC/5689/2020, UIDB/00618/2020 and UIDP/00618/2020.

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Self-assembly and phase separation of cellulose nanocrystals under capillary confinement

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Keywords: cellulose nanocrystal, self-assembly, chiral nematic, capillary

Geometric confinement can guide the formation of hierarchical nanostructures formed by self-assembling lyotropic liquid crystals (LCs) within biological systems.[1] Colloidally stable nanoparticles confined to capillaries result in structures mimetic of those observed in nature and may be useful for understanding the fundamental self-assembly process or the development of new technologies that require long-range order, such as photonic waveguides.[2],[3] Cellulose nanocrystals (CNCs) self-assemble into left-handed chiral nematic (*Ch*N) LC mesophases that have been studied extensively under confinement.[4],[5],[6],[7] However, aqueous suspensions of CNCs may undergo undesirable phase separation or form defects trapped in the *Ch*N structure, which affects their long-range order.[8],[9] In my presentation, I will describe our comprehensive investigations on CNC *Ch*N phase formation, propagation, and separation under capillary confinement over long length scales and time periods.

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Surface Pressure Induced Nanoarchitectonics of Photoisomers of Alkylated Azo-benzene Molecules

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Keywords: (Azo molecule, Self-assembly, Photoisomerisation, Atomic Force Microscope)

Molecules containing the azo group possess intriguing potential for a spectrum of optoelectronic applications owing to their inherent photo-switchable attributes. In this work, the self-assembly of an alkylated azobenzene system has been studied at air-water (A-W) and air-solid interface, and its photo-switching property has been explored. The molecular organization at the A-W interface has been investigatedby measuring surface pressure (π) – area (A), and surface potential(ΔV)-area (A) isotherms, compression- expansion isotherm as well as by Brewster angle microscopy (BAM). It has been observed that the film forms a reversible and stable monolayer at the A-W interface and exhibits a liquid condensed phase even in its most compact form. The molecules show reversible trans-cis photoisomerization in the solution when irradiated with UV and visible light alternatively, as confirmed by UV-visible absorption spectroscopy. UV irradiation causes an increase in mean molecular area and collapse pressure of the film at the A-W interface. Atomic force microscope (AFM) topography images of the film transferred onto Si substrates show the formation of uniform compact films. The ability of the molecule to be transferred onto solid substrates and become stable and uniform makes it suitable for several nano-device applications, especially for optoelectronics and photoswitching.

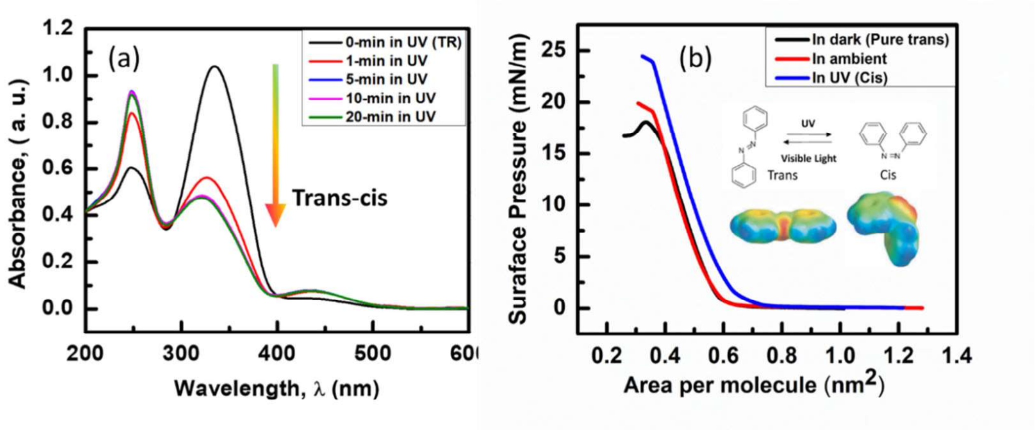

Figure 1: (a) UV-visible absorption spectroscopy (b) π- A isotherm of the molecule under different light irradiation conditions.

Acknowledgements: We acknowledge IIT Patna for research facilities. P.P.S. acknowledges PMRF funding (PMRF-ID: 2702446) for her research fellowship.

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The physicochemical characterization of phosphatidic acid and diacylglycerol pyrophosphate interactions.

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Keywords: lipid-lipid interactions, lipid domains, solid state NMR, membrane physical chemistry.

Phosphatidic Acid (PA) is an anionic lipid with numerous signaling functions in bacterial, animal, and plant cells. PA is converted to diacylglycerol pyrophosphate (DGPP), a lipid second messenger, during stress signaling in plants, fungi, and some parasites. DGPP differs from the cone shaped PA by having a higher charge and zero curvature at physiological pH [1]. DGPP is therefore expected to affect membrane properties and interactions with proteins differently from PA. However, the specific functions of DGPP in the signaling pathway are yet to be established. The ionization properties of PA and DGPP have each been shown to be affected by intermolecular hydrogen bond formation with vicinal lipids and protein-lipid interactions [1-4]. Hence, it is possible that PA and DGPP interact together to affect each other's biophysical properties. In this study, we use ^{31}P MAS NMR to determine the effect of PA and DGPP interactions on each other's ionization properties in model membranes made of equal concentrations of phosphatidylcholine and phosphatidylethanolamine. Our results show that the charge on PA and DGPP decreases with increasing concentration. Interestingly, this charge is higher than in systems where just PA or DGPP is present in the membrane. These results thus suggest that PA and DGPP interact in the membrane, possibly by domain formation via hydrogen bond interactions. Such interactions may impact the individual associations of PA and DGPP with proteins to modify intracellular signaling pathways.

Acknowledgements: partially funded by National Science Foundation (USA) grants 1412920 and 1457873.

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E5

Biological sensors – Organic electrochemical transistors, etc

Development of label-free biosensor using liquid crystal droplets for detection of amyloid beta-42

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Keywords: Nematic droplets (NLC), Alzheimer disease, Aβ1-42, Anti-Aβ1-16,antigen, Phosphate Buffer Saline (PBS).

Abstract

The liquid crystal droplets in aqueous solution have emerged as optical probes for sensing the absorption and interaction of biological analyte at the LC surface. In this work, we report an immunoassay in which Purified anti-β-Amyloid, 1-16 Antibody (Anti-Aβ1-16) are immobilized on the surface of nematic liquid droplets (NLC) treated with Poly ethylenimine (PEI)/Tween-20, when we incubate the LC droplets immobilised Anti-Aβ1-16 in a solution containing Amyloid beta1-42(Aβ1-42) antigen droplets changes their orientation from radial to bipolar. In Contrast, when droplets immobilised antibody/antigen no changes were observed. the shift in orientational arrangement indicates the creation of an immunocomplex Anti-Aβ1-16 with Aβ1-42 on the surface of the LC droplets. Our results show the use of the director configuration of NLC droplets as an optical probe to observe antibody-conjugate antigen interactions at LC/aqueous interfaces and might be used to construct a biosensor for in vivo detection of proteins and pathogens in aqueous medium.

Acknowledgements:

The authors would like to thank the Department of Physics and the Central Research Instrumentation Facility (CRIF) at NIT Warangal for providing research facilities. The authors thank Department of Biotechnology, New Delhi, India for providing financial support in the form of Research grant No: BT/PR35841/MED/32/745/2020.

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Highly sensitive and Non-specific Sensing of Proteins using Microdroplets from Light treated Nematic Liquid Crystals

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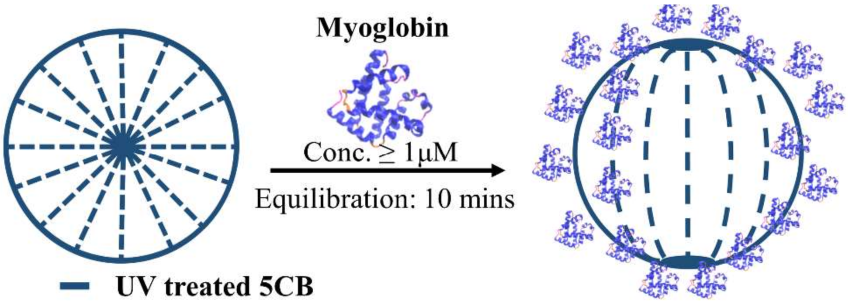
Protein detection at low concentrations is fundamental to many biomedical and industrial applications due to its utilization in drug discovery, prevention of infectious pandemics, etc.[1] Established methods involve surface immobilization of proteins of interest onto a solid surface or by bringing them in contact with a labeled stimuli-responsive interface. However, these detection techniques require sophisticated and complex instrumentations. In my presentation, I will talk about a generic, sensitive, and label-free method for protein detection at the interface of nematic liquid crystal (LC) droplets and the aqueous phase. Nematic liquid crystals have several technological applications and have been used for sensing various analytes like surfactants, lipids, etc. However, their use as protein detection elements in optical biosensors depends on co-nematogens or biomolecular surface modifications. Using UV-treated 4-cyano-4′-pentylbiphenyl (5CB) nematic LC, we prepare highly monodisperse (diameter: 20μm) droplets using a flow-focused microfluidic device that exhibits the radial defect optical configuration due to the homeotropic anchoring of LC molecules with respect to the interface.[2] An aqueous solution of proteins (α-Syn, α-CT, Mb, or BSA), triggers a radial to bipolar transition of 5CB molecules within the droplets due to a non-specific, electrostatically mediated adsorption at the LC-aqueous interface. The proteins could be detected at low concentrations of ~ ≥ 25nM. Our results also indicate the dependence of the detection limit on LC droplet, protein charge, and LC droplet concentration. This generic and highly sensitive LC droplet-based sensing method holds promise for cost-effective, rapid, and easy protein detection at ultra-low concentrations.



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Liquid crystal based sensor for the detection of Cr^{3+}, Cd^{2+}, Zn^{2+} and Pb^{2+} ions in water

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Keywords: Liquid Crystals, sensors, heavy metals

Heavy metal ions are among the most dangerous water pollutants. In this work, we are focused on the development of label-free and real-time liquid crystal-based sensors for the detection of heavy metal ions in water samples. Nematic liquid crystal (LC) 4-pentyl-4'-cyanobiphenyl (5CB) is used as a platform to create an LC-aqueous interface placed into the TEM grids. This system enabled the detection of metallic ions in solution such as Cr^{3+}, Cd^{2+}, Zn^{2+}, Pb^{2+}. Detection relies on the orientation transitions of liquid crystal molecules that are transmitted through optical signals when using polarized light microscopy. When the solution was incubated into the system, particular morphologies in the image were observed, shifting from a dark to a bright optical image, signifying a transition from a planar to a homeotropic orientation. This change indicates that upon contact with the metallic ion, the orientational order is disrupted.The implementation of this method provides an effective tool for the real-time detection of metallic ions in water samples, proving to be important for addressing the issue of water pollution by heavy metals.

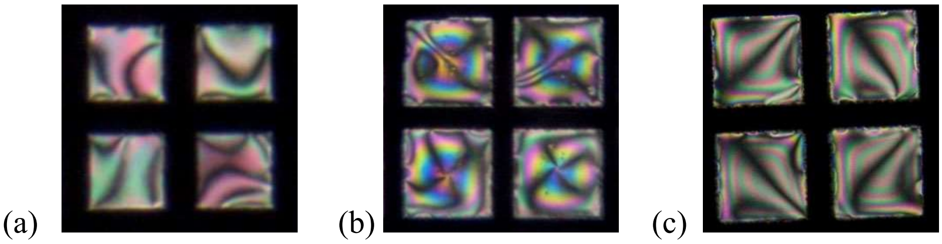

Figure 1: Polarized images of 5CB filled grids immersed in aqueous solution containing different heavy metal ions: (a) Zn^{2+}, (b) Cd^{2+} and (c) Pb^{2+}.

Acknowledgements: Mariana V. Morales-Rodriguez acknowledges to CONACYT for scholarship support. Julio C. Armas-Perez acknowledges to University of Guanajuato for its financial support through the Project CIIC 267/2023.

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E6

Lyotropic system and instrumentation

Comparison of Liquid Crystalline Phases of DNA Sequences G_4C_2 and $(G_4C_2)_2$

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Keywords: Liquid Crystals, Polarized Optical Microscopy, DNA, DNA-Quadruplexes

Research conducted in the 1980s showed that DNA forms lyotropic liquid crystalline (LC) phases in concentrated solutions [1]. More recently, it was found that LC phases are also formed by short segments of DNA that stack on top of each other and form rod-like assemblies [2], enabling the formation of nematic and columnar LC phases – a noticeable feature of chromonic systems. In our research, we studied two short guanine-rich DNA sequences, G_4C_2 and $(G_4C_2)_2$. These sequences form higher-order structures, including G-quadruplexes, in addition to the well-known double helix conformation. DNA G-quadruplexes are integral to the regulation of genes and play a significant role in diverse cellular processes. DNA sequences G_4C_2 and $(G_4C_2)_2$ are known for their involvement in neurodegenerative diseases, especially amyotrophic lateral sclerosis (ALS). In previous research, we used dynamic light scattering (DLS) and atomic force microscopy (AFM) to confirm that both sequences form G-quadruplexes [3]. We also determined their length: sequence G_4C_2 forms long aggregates, with lengths of more than 80 nm, while sequence $(G_4C_2)_2$ forms short quadruplexes, approximately 3 nm in length. Due to its extreme length, stacked G_4C_2 is an excellent candidate for the formation of chromonic LC phases. We prepared concentrated aqueous solutions G_4C_2 and $(G_4C_2)_2$ and studied them by polarization optical microscopy (POM). At the minimum concentration needed for the formation of LC phases, both sequences formed islands of columnar LC phase surrounded by isotropic solution. The LC textures for G_4C_2 and $(G_4C_2)_2$, however, were markedly different (Fig. 1) and correlated to the length of the G-quadruplex assemblies. This is a feature typical for chromonic systems, where the LC formation is controlled not only by temperature but also by solution concentration and the extent of stacking interactions.

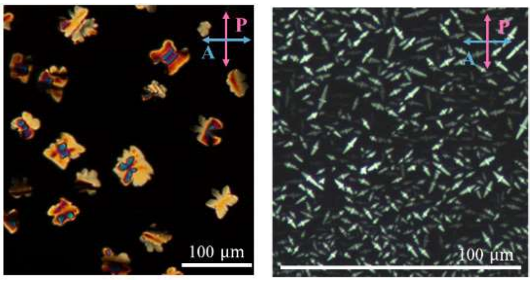

Figure 1: Columnar LC phases in isotropic environment for DNA sequences G_4C_2 (left) and $(G_4C_2)_2$ (right).

Acknowledgements: This work was supported by the Slovenian Research Agency in the framework of research program P1-0192.

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Frequency dependence of the dielectric response of graphene oxide liquid crystal

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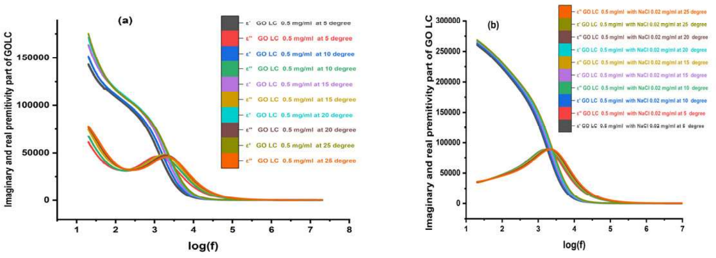
Keywords: Graphene oxide, Dielectric spectroscopy, Permittivity, Sodium Chloride, Liquid crystals

Graphene Oxide (GO) can easily form a liquid crystal phase by dissolving very low concentrations of GO flakes in water which is highly attractive for investigating its application in many areas such as low-energy, electric and electro-optical devices like LCDs [1]. Its distinctive phase formation properties are attributed to the presence of hydroxyl, epoxide, carbonyl, and carboxyl functional groups on the graphene flakes as well as to the ionic strength and PH of the dispersion [2]. The dielectric permittivity depends on the graphene flake characteristics, including the presence of functional groups but also on the ionic contribution and clearly on the flake concentration. Here, we report a thorough study of the impedance of GO liquid crystal for determining the different contributions to the dielectric constant and their impact in the investigated frequency range, from 20 Hz to 20MHz, using specially prepared cells. In the figure. below we report the dielectric spectra of GO LC in the pristine form and with the addition of NaCl (0.02 mg/ml) as function of temperature. The presence of NaCl increases the low frequency value of the real permittivity of GOLC while pushing. to lower frequency the imaginary primitivity relaxation peak. The full spectra are fitted with circuital models in order to determine the values of the physical components contributing to the frequency-dependent dielectric response.



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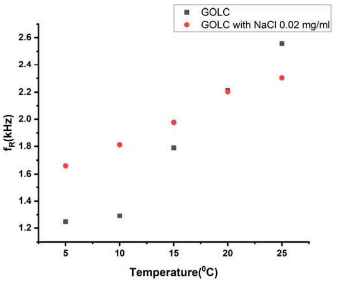

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Figures 1) Temperature-dependent real and imaginary permittivity of (a) GOLC, and GOLC with 0.02 mg/ml NaCl (b).
2) Temperature dependence of the relaxation frequency f_R of pristine (black) and of GO, with 0.02 mg/ml NaCl (red).

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Liquid Crystals as Sustainable Phase-Changing Materials in Textile Engineering

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Keywords: Phase-Changing Materials, Liquid Crystals, Smart Textiles, Environmental Footprint, Sustainable Development

The contemporary stance of the textile industry towards fast fashion today represents a trajectory leading toward an impending ecological disaster. This mode of production has a significant impact on the environment, as every stage of the process consumes a considerable amount of fresh water, materials, chemicals, and energy resources [1]. In our research, we investigate the use of phase-changing materials (PCMs) in textiles, a topic that has gained considerable attention in recent years, particularly in the development of smart textiles capable of responding to external stimuli [2]. These textiles can actively regulate heat transfer, providing enhanced comfort and functionality for the wearer. Our focus is on liquid crystals as an innovative option. Liquid crystals (LCs) exhibit diverse mesophases that are temperature-dependent and display a significant response to minor external perturbation [3]. Through theoretical modeling, we demonstrate the factors affecting the release or absorption of latent heat. Furthermore, we study the ecological aspects of integrating PCM textiles and compare the environmental impact between LCs and commonly used PCMs. The primary objective of our study is to understand how the use of these materials reflects on sustainability and the environmental footprint. We are committed to developing sustainable solutions and reducing negative impacts on the environment. Our research goes beyond technical aspects, emphasizing the significance of sustainable design in the context of textile innovation. By combining theoretical approaches with practical trials, we aspire to contribute substantively to a better understanding and implementation of PCM within the textile industry.

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Nanosheet synthesis using hyperswollen lamellar phases

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Keywords: Hyperswollen lamellar phase, Industrial production, Nanosheets

Nanosheets are a type of nano-structured materials that exhibit quantum size effects. Since their widths are more than 100 times larger than their thickness, they are easy to separate. They have been synthesized mainly by top-down exfoliation methods. They can now also be synthesized by bottom-up methods such as chemical vapor deposition and hydrothermal synthesis. Recently, various interfaces and layer structures have been used as templates to obtain thin nanosheets of non-layered materials [1]. A new bottom-up method using lyotropic lamellar phases has been reported [2], but it tends to produce thicker particles (tens of nm) due to the high concentration of raw materials. For synthesizing highly dispersed thin nanosheets, the spaces between two-dimensional templates should be wider. If this can be achieved, it should be advantageous for subsequent adsorption and coating processes.

Hyperswollen lamellar phases consist of periodically separated amphiphilic bilayers at intervals of several hundred nanometers. In general, an appropriate volume ratio of the hydrophobic and hydrophilic parts of the amphiphiles is required to exhibit the hyperswollen lamellar phases. We have developed the two-dimensional reactor in amphiphilic phases (TRAP) method, a nanosheet synthesis method using the hyperswollen lamellar phase as a template. Here, after a broad introduction of the advantages and applications of the TRAP method [3-5], we report in detail the synthesis of amorphous aluminosilicate nanosheets using liquid crystals as templates [6,7].

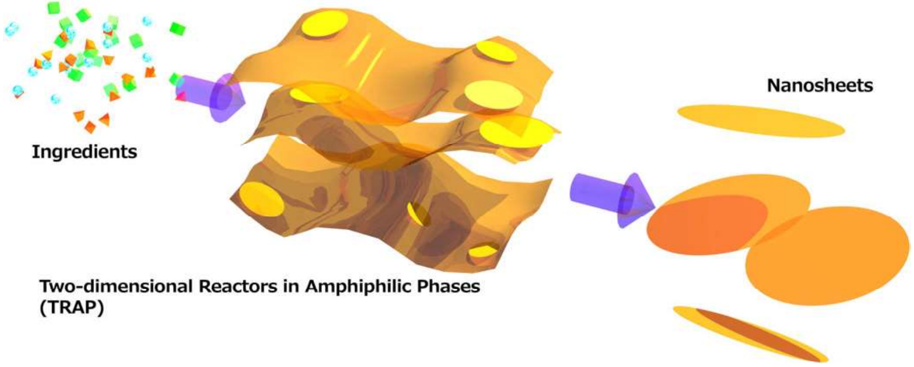

Figure 1: Schematic illustration of TRAP method.

Acknowledgements: JSPS KAKENHI (JP22H04477, JP22H02158)

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Stabilization of water-in-water emulsions by interfacial lipid self-assembly

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Keywords: water-in-water emulsion, lipids, interfacial self-assembly, lyotropic lamellar phase

Water-in-water (W/W) emulsions produced by liquid-liquid phase separation in aqueous polymer solutions have received an increasing attention for micro-encapsulation applications. Easily produced without oil or organic solvents, these emulsions capture and accumulate various solutes, including biomolecules. However, these emulsions are thermodynamically unstable and tend to a macroscopic phase separation. Molecular surfactants, used to stabilize water/oil emulsions, are inefficient for W/W emulsions. Since fifteen years, many works have tried to tackle this issue. Even though different approaches are effective, they produce highly permeable shells that only partially restrict the diffusion of encapsulated solutes. The main objective of this work is to develop a new, simple and robust stabilization strategy for W/W emulsions with impermeable membranes by interfacial lipid self-assembly.

We formulated model W/W emulsions between poly(ethylene glycol) and dextran in the presence of a small amount (less than 0.5 w%) of lipids and co surfactant. A completly new stabilization mechanism were identified with the coating of droplets by lyotropic swollen lamellar phases. Unexpectedly, the membrane is made of several layers of lipids bilayers separated by a layer of polymer solution, like an onion. A unique formulation route is also described by emulsification of two lamellar phases, doped respectively with poly(ethylene glycol) and dextran solutions and at the dilution limit with their own excess of solvent.

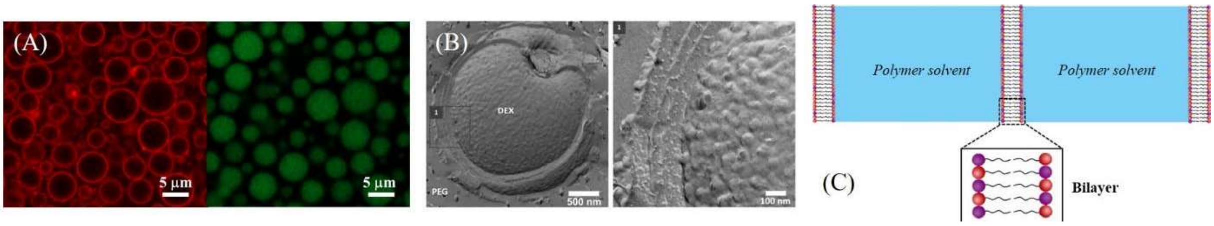

Figure 1: (A) Confocal fluorescence microscopy images (left) Lipids are stained with Nile Red and (right) Dextran droplets are stained with FITC-dextran. Scale bars, 5 µm. (B) Freeze-Fracture TEM showing a Dextran droplet coated by a stack of bilayers. (right) Zoom of the same droplet. Scale bars, 500 nm (left) and 100 nm (right). (C) Schematic representation

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Thermal response of low-density lipoproteins measured by Z-scan in visible and near infrared regimes.

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Keywords: lyotropic-like micellar structure, thermal effect, z-scan technique.

Among biological materials, lipoproteins have aroused the interest of several studies due to their relationship with health-related topics such as cardiovascular disease. Lipoproteins are complex particles that have a central hydrophobic core (non-polar lipids, cholesterol esters and triglycerides) surrounded by a hydrophilic shell (phospholipids, free cholesterol, and apolipoprotein). Low-Density Lipoprotein (LDL) are the main carrier of cholesterol in the human body and when LDL particles are dispersed in water the system can be seen as a lyotropic-like micellar structure. The modification of LDL by oxidation, a gradual process, is one of the first events in atherosclerosis (disease of the arteries characterized by the deposition of plaques of fatty material on their inner walls).

Z-scan technique performed with visible light (532 nm) in millisecond exposition configuration, has been used to characterize parameters related to lipoproteins response to oxidation process [1, 2]. It has been observed that thermal effect invariably decreases with the degree of oxidation of the sample. When z-scan measurements are performed on aqueous LDL samples using 532nm light, lipoproteins absorb the light and transfer heat to the water that has negligible optical absorption at this wavelength ($\alpha_{532nm} \approx 6x10^{-4}cm^{-1}$). When measurements are carried out with IR light (979nm), water absorbs the light ($\alpha_{979nm} \approx 5x10^{-1}cm^{-1}$) and transfers heat to the other components of the sample, changing the dynamics of the heating process.

In this work we will initially show a comparison of the thermal effect magnitude (θ) behavior for non-oxidized samples and with different oxidation times obtained with visible and IR light. For IR measurements, it will be also presented the behavior of the characteristic thermal lens-formation time (t_{c0}) according to the oxidation time of the LDL samples [3]. Besides it will be presented thermodiffusion (exposure on the order of tens of seconds resulting in sample mass displacement) results for oxidized and no oxidized LDL samples.

Acknowledgements: National Council for Scientific and Technological Development (CNPq), Coordination for the Improvement of Higher Education Personnel (CAPES), National Institute of Science and Technology Complex Fluids (INCT-FCx), São Paulo Research Foundation (FAPESP).

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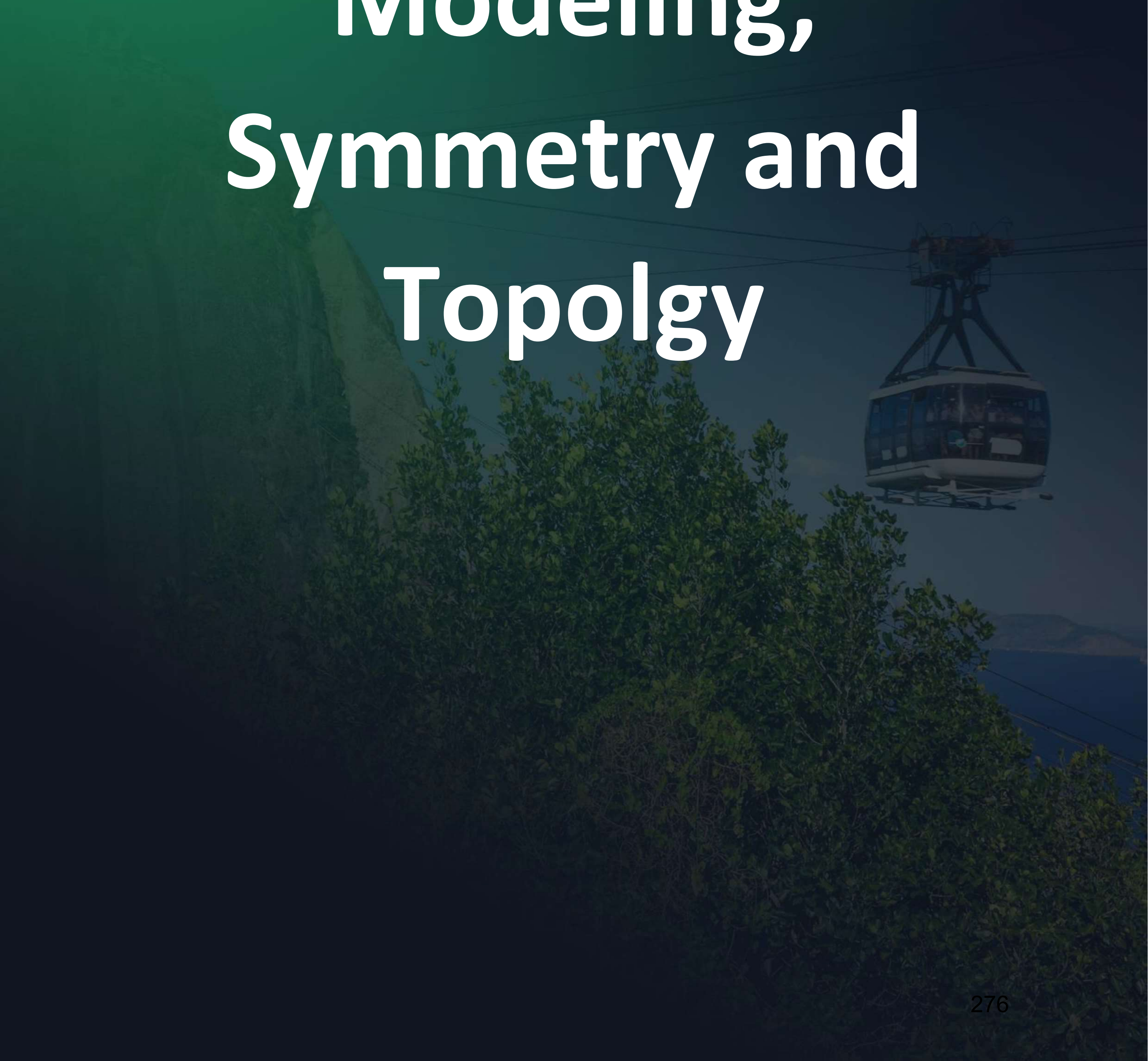
F

Mathematical Modeling, Symmetry and Topolgy



F1

Theory, simulation, and modeling

Activity-induced self-constraint of nematic defects and flow structures

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Active nematics exhibit spontaneous flows with complex spatiotemporal structure. In bulk, disorderly dynamics arise due to the coupling between nematic deformations and active flows, and are characterized by steady-state populations of half-integer topological defects. This talk will demonstrate that, despite their disorderly dynamics, there exists a strong self-constraint that arises between the self-propulsion of motile defects and mesoscale flow structures. Through a combination of microtubule/kinesin-based experiments and nematohydrodynamic simulations, we show that self-motile defects are tightly constrained to particular flow structures where vorticity and the strain rate are balanced, called viscometric surfaces. Although this is consistent with models for the flows generated by isolated +1/2 defects that predict the defect resides at an intersection between two crossing viscometric surfaces, experiments and simulations show that +1/2 defects are predominantly found on a single viscometric surface — only fleetingly passing through intersections — and, thus, possess broken-mirror symmetry. Through a series of simple models, we explain that this spontaneous self-constraint arises from an interdependence between viscometric lines and elongated narrow bend walls in the director field. We provide evidence that this result is not limited to bulk turbulence but occurs whenever self-motile defects are present. These results underscore the continual role of bend walls in steady-state dynamics, showing that active nematic defects cannot be viewed as solitary points but are one component of mesoscale nematic structures, which suggests potential new avenues for exploring topological dynamics.

Figure 1. Experimental snapshot of +1/2 (green comet) and -1/2 (blue trefoil) nematic defects following the borders between vorticity and strain-rate dominated regions of the velocity field. Red borders enclose a clockwise vortex and blue for an anticlockwise vortex.

Anomalous dynamic scaling of an active particle embedded in a smectic liquid crystal

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Keywords: Smectic liquid crystals, Active Brownian Particles, Focal Conic Domains

Self-propelled (active) swimmers exhibit fascinating dynamic behavior with relevance to a wide range of disparate systems found in biology, chemistry, and physics [1]. When embedded in a smectic liquid crystal, swimmer trajectories are affected by layer fluctuations that ultimately lead to anomalous logarithmic tails for the transverse mean-square displacement at long times [2]. This anomalous behavior is different from what is observed for isotropic or nematic fluids, thus motivating us to extend the analysis of Ref. [2] to include the effects of complex smectic microstructures that are produced in diverse protocols. Here we discuss preliminary results, where we use numerical simulation data of Refs. [3,4] to investigate the anomalous dynamic behavior of an active particle embedded in a smectic liquid crystal, with focus on the interplay between activity, flow instabilities and focal conic domains.

Acknowledgements: YMA thanks financial support from CNPq. DBL thanks financial support through FAPESP grants # 2021/14285-3 and # 2022/09615-7.

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Architecture and Inverse Design of Nematic Disclination Lines

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Keywords: Topological Defects; Disclination Lines; Inverse Design

Achieving versatile control over the paths of disclination lines is key to developing novel electro-optical devices, programmable origami, directed colloidal assembly, and controlling active matter. Here, we introduce a theoretical framework that allows tailoring three-dimensional disclination architecture in nematic liquid crystals. By drawing an analogy between nematic liquid crystals and magnetostatics, we produce quantitative predictions for the connectivity and shape of disclination lines found in nematics confined between two thinly spaced glass substrates with strong patterned planar anchoring. We verify our predictions in experiment and in computer simulations, and find nondimensional parameters enabling us to match results at different length scales. We identify critical material parameters that tune disclination paths and allow achieving exact desirable path changes in situ. Our work provides a powerful method to understand and practically control defect lines in nematic liquid crystals.

Figure 1: Heart-shaped disclination lines [1].

Acknowledgements: This research was supported the United States–Israel Binational Science Foundation (Grant No. 2018380) and by the Israel Science Foundation (Grant No. 2677/20).

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Chiral active matter is both `odd’ and non-reciprocal

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Keywords: (rotational active matter, odd viscosity, non-reciprocal)

Active materials are composed of many components that convert energy from the environment into directed mechanical motion, thus locally breaking time-reversal symmetry (TRS). Examples of active materials are numerous, from living systems such as bacteria to colloidal rollers. A striking phenomenon of breaking TRS is the possible appearance of *odd viscosity*. The Onsager reciprocal relations require that, when TRS holds, the viscosity tensor is symmetric for exchanging its first and last pair of indices. However, when TRS is broken in equilbrium systems, Onsager relations predict an *odd viscosity* that is both odd under TRS and under the interchange of indices. Such odd viscosity is non-dissipative and should thus be derivable from a Hamiltonian theory. This talk will discuss *chiral active materials* in which both parity and TRS are broken at the microscale. This is usually a result of continuous injection of energy and angular momentum through local torques, which are abundant in living systems, and generically result in odd viscosity, even when the constituents are non-interacting. Our treatment is closely related to that used in the derivation of the hydrodynamic equations for nematic liquid crystals [1] whose microscopic energy starts with separate kinetic energies for translational and rotational energy of each particle and interactions between pairs of particles. Both of these energies are coarse-grained, and dynamical equations are derived using Poisson brackets. The principal difference between this active model (AM) and the equilibrium one is the spin agular-momentum (SAM) has local spin angular-momentum density (SAMD), forced by a coupling to an external torque, that is non-zero throughout a sample. The mere existence of SAMD breaks Onsager’s reciprocity relations [2] and leads to a non-Hermitian dynamical matrix. When interactions are included phenomenologically, there are regions in the parameter space in which novel 3D mechanical waves propagate in the bulk and regions in which they are mechanically unstable. The boundaries separating these regions are continuous lines of exceptional points, suggesting a non-reciprocal phase transition. The techniques used to arrive these results are easily generalized to treat other rotating systems such as a nematic phase with spinning particles.

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Coarse-Grained Modeling of Ionic Liquid Crystals: Understanding Phase Transitions and Ionic Conductivity

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Keywords: Ionic Liquid Crystals, Ionic Conductivity

Solid-state electrolytes are currently being explored as a safe material capable of addressing consumer energy-storage demands. Solid polymer electrolytes, in particular, offer a high energy density and improved safety when compared to liquid-based electrolytes, but tend to have a significantly lower ionic conductivity. We hypothesize structured, polymerized ionic liquids can enhance conductivity. Here, we explore the performance of these materials through coarse-grained molecular dynamics simulation. While we observe similar phase behavior (incorporating solid, smectic, and liquid phases) to that seen in experiments, we also observe counterintuitive behavior in the conductivity, which we hypothesize is due to specific chemical effects. We further discuss how the general results within this paper can guide further studies and target the design of new highly conductive solid electrolytes.

Coarse-grained simulations of the flocking of active skyrmions

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Keywords: Liquid-crystal skyrmions, Active matter

Motivated by recent experimental results [1] that reveal rich collective dynamics of thousands-to-millions of active liquid-crystal skyrmions we developed a particle-based model to study the “flocking” dynamics of these active skyrmions. The basic physical mechanism of the skyrmion motion is related to the “non-reciprocal” rotational dynamics of the LC director field when the electric field is turned on and off. Using a data-driven approach from numerical results of the continuum model of liquid crystals using the Frank-Oseen formalism, we have mapped this “non-reciprocal” motion to an effective force acting asymmetricaly when the electrical field is on or off. We were able to reproduce motion of the skyrmion given by the continuum model, and we were able to mimic the experimental results showing that the direction and velocity of the skyrmion depend on the frequency of the on/off cycle. We adapted this particle-based model into Langevin dynamics simulations to be subsequently used to model the experimental limit of thousands-to-millions of skyrmions [2]. We have coupled a dipole interaction between skyrmions with this “non-reciprocal” dynamics. We studied a competition between a dipole interaction due to the presence of the field and an isotropic interaction always present between skyrmions. We showed that the structures of clusters of skyrmions can change from chain-like to compact depending on the frequency of the electric field.

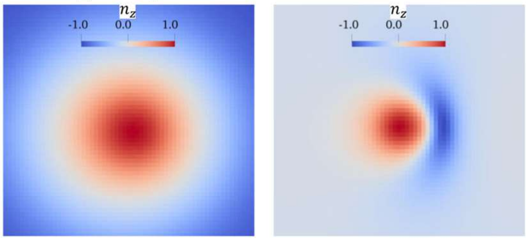

Figure 1: Equilibrium director configurations. (a) Zero external electric field, and (b) electric field of 3.5V.

Acknowledgements: We acknowledge financial support from the Portuguese Foundation for Science and Technology (FCT) under Contracts no. PTDC/FIS-MAC/5689/2020, EXPL/FIS-MAC/0406/2021, CEECIND/00586/2017, UIDB/00618/2020 (https://doi.org/10.54499/UIDB/00618/2020), and UIDP/00618/2020 (https://doi.org/10.54499/UIDP/00618/2020).

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Colloids behavior in the 3D nematic liquid crystal domain under electrical field

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Keywords: Nematic liquid crystal, Lattice Boltzmann method, colloid transport, electrical field, 3D liquid crystal field.

The transport characteristics and the agglomeration behavior of the colloidal particles under electrical field perturbations dispersed in a nematic liquid crystal (NLC) which differs from its isotropic counterpart due to its long-range orientational ordering of the liquid crystal (LC) molecules is explored. The liquid crystalline order is distorted in the presence of the colloids, leading to the formation of the defects[1,2] when minimising the free energy as shown in the figure 1. Because of the anisotropy of the NLC and long range (non-linear) inter-particle interaction, the migration characteristics are different here. When the LC domain is subjected to an electric field, the critical field strength required for the Freedericksz transition (the transition where the LC molecules get aligned in the direction of the applied electric field) is affected due to the presence of the colloids. We performed numerical simulations in three dimensions[3] using the lattice – Boltzmann method[4] and Beris – Edwards model of the nematohydrodynamics to quantify the effect of the electric field on the director field and the defect formation coupled with the Nematohydrodynamics and multibody dynamics.

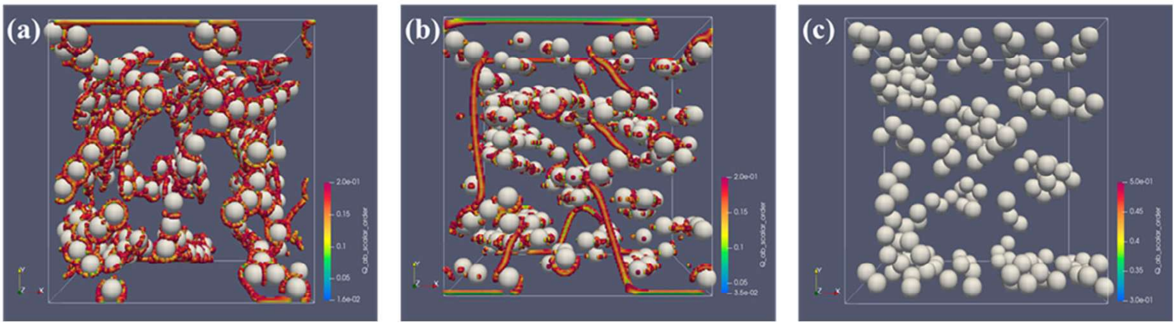

Figure 1: Defect formation around the colloids in the LC domain for the colloidal compositon of 200 colloids of radius 8 (volume fraction = 0.0536) simualtion units for externally imposed different electric field strengths (a) 0 (b) 0.01 (c) 0.14 simulation units.

Acknowledgements: This work was supported by a grant from the science and engineering research board (SERB), Department of science and technology, Government of India, Sanction order: CRG/2021/001218, dated December 30, 2021.

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Complementary tensorial measures of disclination line winding character

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Keywords: disclinations, nematics, topological defects, data analysis

Whereas disclinations in two-dimensional nematics have quantized, half-integer winding numbers, the disclination lines of three-dimensional nematics are much more complicated: The nematic director winds about a rotation vector that can vary continuously in time and along the defect's contour, resulting in a family of winding characters ("wedge", "twist", and their intermediates). This poses challenges for characterizing disclination lines in nematic orientation fields from experiment or simulation. Recently, a second-rank tensorial calculation was proposed that allows the rotation vector to be determined from the orientation field in the vicinity of a disclination.[1] Here, we demonstrate that the rotation vector can also be calculated from an alternative measure, based on a second-rank pseudotensor defined on either the director field or the Q-tensor field.[2,3] We also explore how these measures are connected with saddle-splay and twist distortions as (pseudo-)scalar measures of disclination winding character, and demonstrate their usefulness in large datasets.

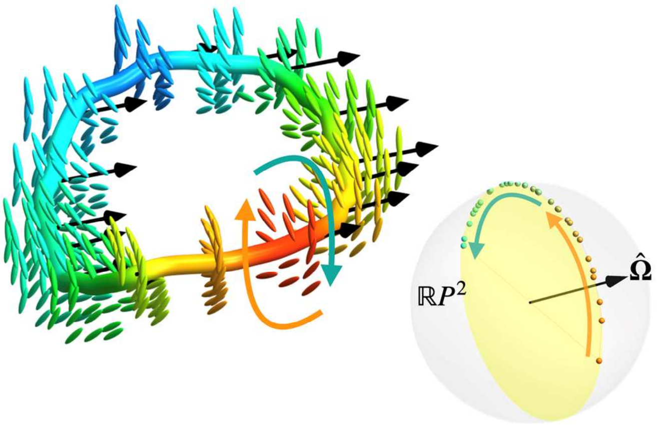

Figure 1: Director field profiles and rotation vectors (black) on a simulated disclination loop (left) and corresponding map in order parameter space (right) at one point.

Acknowledgements: This material is based upon work supported by the National Science Foundation under Grant No. DMR-2225543.

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Controlling reflection and absorption of antennae array in THz using liquid crystals and a liquid crystal elastomers

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Keywords: dipole antenna, Yagi-Uda antenna; liquid crystal; liquid crystal elastomer; controllable reflection and absorption; metamaterials.

In this study we explore the possibilities of tuning dipole and Yagi-Uda antennae arrays operating at terahertz frequencies (THz). In the case of dipole antenna array, we use a liquid crystal elastomer to reversibly change the reflection and absorption of the array by applying a strain to the elastomer filled with metallic dipoles. The stretching of the liquid crystal elastomer induces changes in the periodicity and thickness of the system, ultimately modifying the reflectance and absorbance. A linearly polarized wave is either normally or obliquely incident onto the antennae array. In the case of the Yagi-Uda antennae array the structure under investigation comprises a 2D array of metallic Yagi-Uda antennae on a dielectric substrate with a continuous metallic film below and a vacuum layer further beneath. Above the antennae array, there is a layer of nematic liquid crystal (LC) with the initial pi/2 twist of the LC director. Under the Mauguin regime the light polarization rotates following the LC director rotation. The application of an external electric field perpendicular to the substrates reorients the liquid crystal director from its initial twisted state to a homeotropic state, resulting in a change in the light's polarization upon reaching the antennae array.

Our investigation revealed that varying the strain applied to the LC elastomer or voltage applied to initially pi/2 twisted nematic allows for the tunability of plasmonic resonances within the antennae array in the mentioned metamaterial structures. The tunability covers a frequency interval of approximately 7–12 THz. The incident intensity reflectance and absorbance tuning range reaches 90% at some frequencies. By utilizing the electro-optic properties of nematic liquid crystals and elastic properties of LC elastomers, this study introduces a method for tuning the antennae array in THz applications.

Dissipative particle dynamics simulations of photoswitchable surfactants

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Keywords: photosurfactant, simulation, micelles, dissipative particle dynamics

A recently synthesized arylazopyrazole-based photosurfactant [1] has been shown to exhibit complex and interesting phase behaviour upon exposure to UV light. Such surfactants are capable of phase changes due to photoswitching, which results from photoinduced *trans-cis* isomerisation. Photoswitchable phase changes occur across a range of concentrations, including transitions from hexagonal phase structures to bicontinuous and isotropic phases. At lower concentrations (< 30wt.%) micellar phases form, and upon photoswitching micelles transform from oblate ellipsoidal micelles into smaller, spherical micelles. The mechanism behind why these changes occur is difficult to infer from experimental data alone, and hence simulation can help in understanding the observed experimental behaviour.

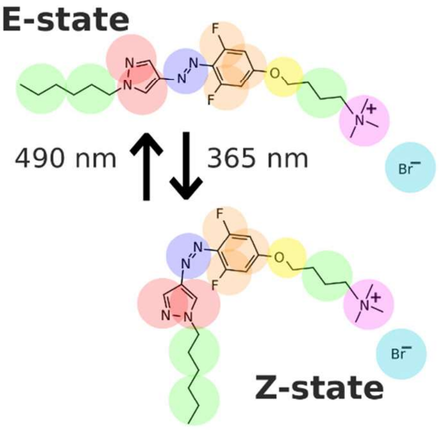

Figure 1: Photoswitchable surfactant with simulation coarse-graining shown.

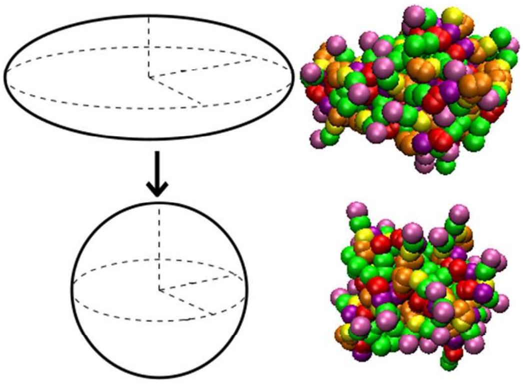

Figure 2: Micelles become more spherical upon photoswitching.

In this work, we investigate these systems using dissipative particle dynamics (DPD) simulations. DPD is a coarse-grained simulation technique which is commonly used to investigate systems which are difficult to study using more detailed methods such as molecular dynamics. We show that we can not only reproduce the observed experimental behaviour, but also provide insight into why phase changes are occurring. The mechanism via how the molecules pack into their various phase structures is easily analysed from our simulated results, as well as quantities such as micelle shape, aggregation number, critical micelle concentrations, along with liquid crystal properties such as periodicity. Understanding the behaviours of such molecules opens the possibility for their use in applications such as photoswitchable membranes.

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Dynamics of Liquid Crystal Skyrmions: Insights from a Collective Variable Model

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Keywords: Driven skyrmions

Liquid crystal skyrmions are topologically protected spatially-localized distortions of the director field which exhibit particle-like properties including translational motion in oscillating electric fields. Here, we develop a collective variable model of the skyrmion dynamics, extending the approach of Long and Selinger proposed earlier for one dimensional system. Our model relates the skyrmion motion to a complex dynamic of the width of the twist wall around the skyrmion core. The width evolves in a non-reciprocal way, quantifying squirming deformations of the high twist region within *on* and *off* states of the field. We discuss the average skyrmion velocity as a function of the frequency, strength and duty cycle of the electric field. The model predictions agree qualitatively with experiments and results of numerical minimization of the Frank-Oseen free energy. Our analysis provides insights into the conditions necessary to observe velocity reversal as a function of the field parameters.

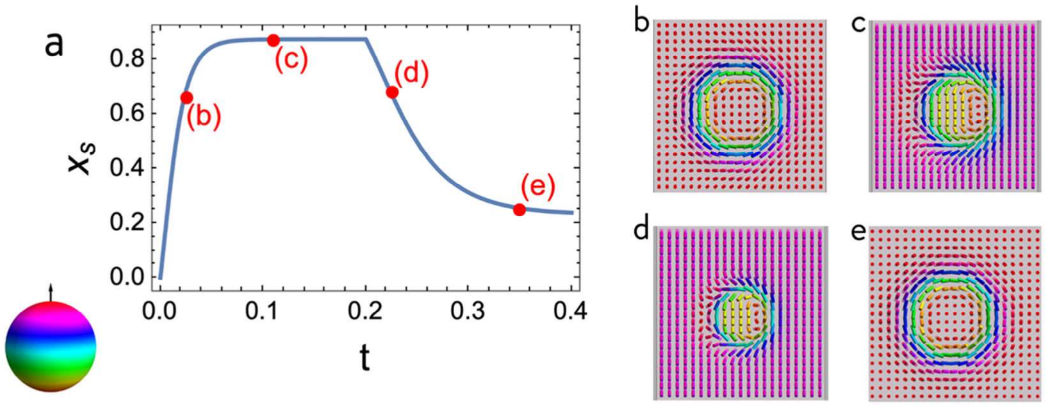

Figure 1: (a) Skyrmion position as a function of time, and (b)-(e) the snapshots of the skyrmion configurations upon turning the field on (at t=0) and off (at t = 0.2). The director field is reconstructed from instantaneous collective coordinates and is shown by cylinders coloured according to their orientations on the surface of a 2-sphere (see bottom-left of (a)).

Acknowledgements: We acknowledge financial support from the Portuguese Foundation for Science and Technology (FCT) under Contracts no. PTDC/FIS-MAC/5689/2020, https://doi.org/10.54499/UIDB/00618/2020, and https://doi.org/10.54499/UIDP/00618/2020.

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Elastomer cholesteric waveguide slab for a transverse elongation

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Keywords: waveguides, elastomer cholesteric, liquid crystals, optical properties.

In this work, electromagnetic propagating modes within a planar waveguide feature a cholesteric elastomer core whose helical axis is oriented perpendicular to the planar boundaries are analyzed. The Maxwell equations and the constitutive equation are used to establish a novel configuration, enabling the tuning of mechanical stress through elastic strain in the perpendicular stretching along the helix axis. The derived set of equations is numerically solved, presuming the waveguide to be surrounded by either air or a vacuum medium. The corresponding band structure and the ratio between electric and magnetic modes have been plotted as a function of angular frequency. The amplitudes of the electromagnetic field profiles are also investigated as functions of position. The ratio of Transverse Electric and Transverse Magnetic modes, along with the cut-off frequencies, are also examined as functions of strain. Finally, the mixing of transverse electric and magnetic modes to generate new eigenmodes, as well as the investigation of their propagation conditions within the waveguide, is examined in the study.

Acknowledgements: This work was supported by the Mexican National Council for Science and Technology (CONACYT) for financing this work through scholarship, 'National Scholarships' (Becas Nacionales). J Adrian Reyes acknowledges partial support from grant Dirección General de Asuntos del Personal Académico UNAM IN100921.

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Externally Controllable Nematic Flow Induced by Active Surface Anchorings

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Keywords: (Active matters, nematodynamics, active surface anchoring, micro-fluids)

Usually, active matters exhibit some sort of nematic order which constantly is distorted due to internal activity of the system. But can this also happen in reverse? Can nematic order distortions cause stable activity in intrinsically passive systems? Well, there is a phenomenon called backflow effect. This means that elastic distortions can cause flux in nematic liquid crystals (NLC). However, to achieve a net flux, the distortions must be induced in a non-reciprocal manner. One of the most effective ways to induce the elastic distortions into the bulk of the NLC is to change the boundary conditions in time and space, which we call active surface anchoring. Our simulations show that if the surface anchoring on the surface non- reciprocally changes in time, e.g., like a wave, there will be a back-and-forth flow with a nonzero time average, as in a heartbeat, which by breaking some system symmetries results in a ***net flow***.

Frank-Read Mechanism in Nematic Liquid Crystals

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Keywords: (Topological Defects, Disclination, Experiment, Theory, Simulation)

In a crystalline solid under mechanical stress, a Frank-Read source is a pinned dislocation segment that repeatedly bows out and detaches, generating concentric dislocation loops. This fundamental mechanism of defect production explains how ductile metals undergo plastic deformation. We demonstrate that, in nematic liquid crystals, an analogous Frank-Read mechanism generates disclination loops. Using experiment, theory, and simulation, we study a disclination pinned between topological defects in the anchoring layer on one substrate in a nematic liquid crystal cell, while the other substrate has planar anchoring. Imposing a twist between the substrates drives lateral motion of the disclination, which bows, self-intersects, and snaps off a new loop as shown via simulation in Fig. 1. The emitted loop expands, with twist inside the loop relaxed by 180°. The original pinned defect remains, and further twist generates more loops. Critical stress for loop emission scales as the inverse of pinned segment length. Frederick Charles Frank (1911-1998) made crucial contributions to the study of crystal plasticity and also formulated the Frank free energy for liquid crystals. This work brings together and builds upon Frank's enduring scientific legacy in both fields. Note: A paper describing our results is accepted/in press at Physical Review X [1].

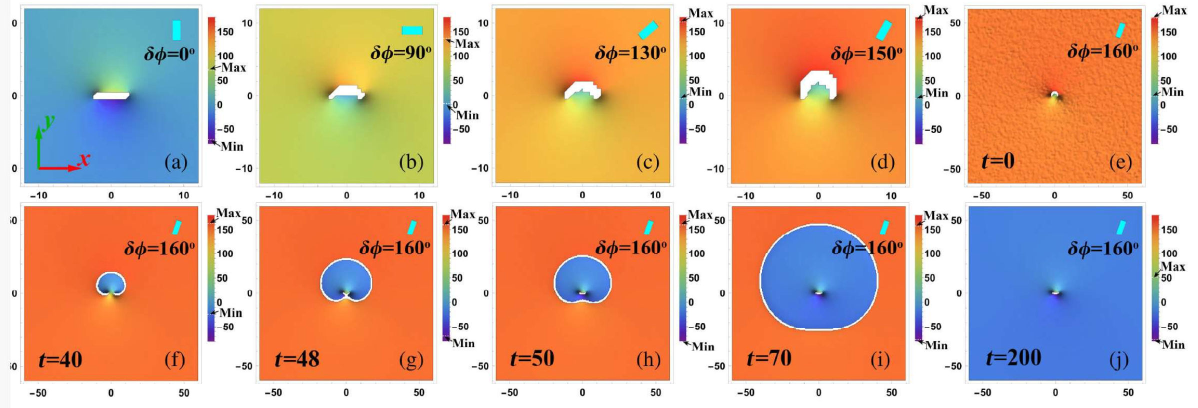

Figure 1: Q-tensor simulation of the Frank-Read mechanism in a nematic cell. A disclination is pinned between +1/2 and -1/2 defects on one substrate, while the opposite substrate has planar anchoring. Imposed twist between substrates drives disclination bow-out, and at a critical angle, a new loop snaps off and expands. Color indicates twist angle between bottom and top surfaces, with (a-d) narrow view (24×24), (e-j) wider view (120×120).

Acknowledgements: Supported by US National Science Foundation CMMI-1663041.

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Inverse Design of Disclination Line Paths and Path Homotopies

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Keywords: Topological Defects; Disclination Lines; Inverse Design

Accurate design and control over the paths of disclination lines is a key element in a variety of technological and industrial applications. In this work we show how to accurately achieve arbitrary two-dimensional paths for disclination lines in a nematic liquid crystal placed between two thinly spaced patterned plates with planar anchoring, building upon the theoretical framework presented in [1]. Using the observation that disclination trajectories are contingent on a dimensionless temperature-dependent material parameter, we investigate the temperature-dependence of paths for given surface patterns. We show that it is possible to inverse-design a pattern to induce a desirable homotopy of disclination paths, namely a different desirable path for each temperature. We discuss conditions for the stability of the solutions and study the role of topological defects in the surface patterns. We demonstrate useful applications of our work for making temperature-responsive disclination-based designs, dials and switches.

Acknowledgements: This research was supported the United States–Israel Binational Science Foundation (Grant No. 2018380) and by the Israel Science Foundation (Grant No. 2677/20).

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LiquidCrystalGLBT.jl: Simulating Lyotropic Nematohydrodynamics with a Julia-Based Solver - Bridging Theory and Computation

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Keywords: Activity, Lyotropic, Hydrodynamics, Julia, Lattice Boltzmann

Controlling active lyotropic Liquid Crystal (LC) experiments, typically an active nematic coexisting with an isotropic fluid and molecular motors providing activity, remains a challenge due to unclear relationships between their component concentrations. This prompts questions about the general conditions and effective parameters transforming their chaotic dynamics into coherent motion. As a result, continuum theory and numerical simulations become essential tools for predicting and guiding such experiments.

Here, we introduce LiquidCrystalGLBT.jl, an open-source Julia-based solver designed for managing the nematohydrodynamic equations of active lyotropic liquid crystals. This hybrid solver combines an upwind finite difference scheme with the Galerkin Lattice Boltzmann method. In our acronym, 'G' indicates the use of the out-of-equilibrium GENERIC framework [1] to derive our equations, while 'LB' signifies the implementation of the Lattice Boltzmann Method through the Trixi.jl package [2], the 'T' in our name. We present three cases stemming from our solutions: 1) A study of a 2D binary mixture, resembling chromonic LC experimental data with +/- ½ topological defects [3]. 2) The introduction of a velocity parabolic profile that distorts an axial LC droplet immersed in an isotropic environment. 3) The addition of biochemical activity, resulting in turbulent simulations flowing naturally, akin to microtubule or actin realizations [4]. Furthermore, we benchmark the performance of our code by increasing the computational nodes.

In short, our findings, achieved through cutting-edge computational and theoretical approaches, showcase the potential predictability of experimental data. This work addresses the challenge of achieving stable and efficient simulations for lyotropic liquid crystals, contributing significantly to our understanding of their dynamic behavior.

Acknowledgements: This work was partially funded by the Chicago Materials Research Center at the University of Chicago under NSF award number DMR-2011854.

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Liquid crystal skyrmions in shear flows

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Keywords: skyrmions; fluid dynamics; topological defects; lattice Boltzmann method; cholesteric liquid crystals.

Liquid crystal skyrmions are topologically protected configurations of the director field formed under confinement between two parallel plates. They can be distorted and displaced, for instance, using an oscillating electric field, but not easily destroyed. Because the medium is liquid, mass flows naturally emerge due to director relaxation and/or applied forces. In this presentation, we address the hydrodynamic effects of a flowing skyrmion in two different cells: Poiseuille-like flow (forced flow between stationary plates) and Couette-like flow (relative uniform motion of the plates). We use lattice Boltzmann simulations in GPU of a 3D domain and experiments to study the dynamics, deformations and stability of the skyrmions. We find that, in Couette-like flows, the skyrmion moves in inclined trajectories with respect to the direction of the plate motion, as a result of local changes in the fluid flow around the skyrmion. For Poiseuille-like flows, the skyrmion distorts and moves at a constant speed under small forcing while it is destroyed by shear under higher forcings. This study is relevant in future lab-on-a-chip applications of display and memory technologies.

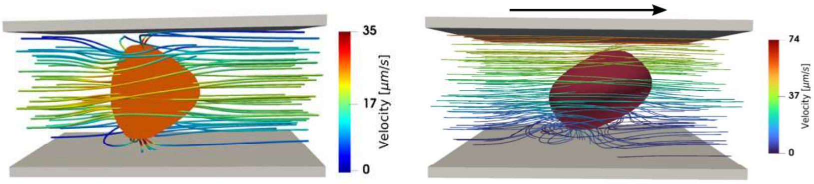

Figure 1: Liquid crystal skyrmion in a Poiseuille-like and Couette-like flow respectively.

Acknowledgements: This work was funded by the Portuguese Foundation for Science and Technology (FCT) under the contracts: PTDC/FIS-MAC/5689/2020, UIDB/00618/2020 and UIDP/00618/2020.

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Mesoscale simulations of nematic colloids: defect structures and transport in complex environments

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Keywords: Topological defects, Numerical simulations.

Colloids dispersed in nematic liquid crystals form topological composites in which colloid-associated defects mediate interactions while adhering to fundamental topological constraints. Better realizing the promise of such materials requires numerical methods that model nematic inclusions in dynamic and complex scenarios. We employ a nematic Multi-Particle Collision Dynamics algorithm (N-MPCD) [1] to simulate colloids as mobile surfaces embedded in a fluctuating nematohydrodynamic medium. We show that N-MPCD resolves elastic interactions between colloids and forms expected defect structures (example shown in Figure 1). We simulate the coarsening dynamics of defect loops from a thermal quench, uncovering metastable states and topological transitions between defect configurations. Hydrodynamic fluctuations enable previously unexplored far-from-equilibrium defect structures to form with positive winding profiles and tilted conformations. Finally, we utilize N-MPCD to model colloidal transport and defect configurations in microfluidic channels with wavy wall geometries. We find that colloidal trajectories undergo stick-slip dynamics due to defect interactions with the confining walls, demonstrating a potential to control intermittent site-specific resting duration. The adaptability and precision of this numerical approach offers promising avenues for studying the dynamics of colloids and topological defects in designed and out-of-equilibrium situations.

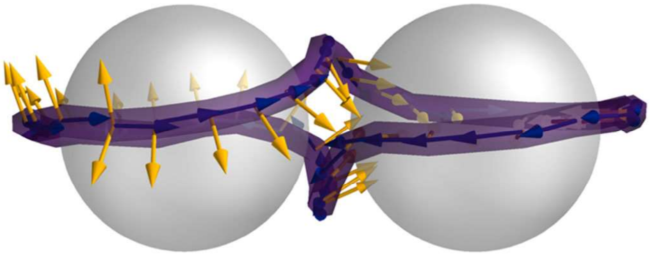

Figure 1: Entangled disclination (purple) accompanying two spherical colloids (grey). Blue arrows indicate the line tangent and orange arrows follow one of the three radial orientations of a -1/2 disclination profile.

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Nanoparticle assembly in smectic-A liquid crystals at undulated surfaces

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Keywords: self-assembly, Landau-de Gennes free energy, colloids, focal conic domains

In a hybrid aligned smectic-A (SmA) liquid crystal, focal conic domains (FCDs) are defect structures that arise to maintain the equal layer spacing of SmA molecules. These topological defects can then be utilized as templates for nanoparticle (NP) assembly. In this work, we model how NPs assemble in a hybrid-aligned SmA liquid crystal, where one of the surfaces has 2D undulations. Using Landau-de Gennes free energy minimization allows us to construct an approximate director field for nonzero eccentricity FCDs in the SmA phase. Independent of their surface anchoring, NPs assemble sequentially: forming a monolayer of NPs on the surface with planar anchoring once the elliptical defects of FCDs are filled, afterwards decorating the hyperbolic line defects then packing on the surface with homeotropic alignment before assembling in the remainder of the LC bulk. We further investigate how the presence of these NP assemblies affects the defect structures arising in the SmA phase.

Acknowledgements: We acknowledge the support from American Chemical Society Petroleum Research Fund Grant #65254-DNI4 and National Science Foundation Grant #DMR-2225543.

Nematic elastomers, relaxation dynamics and active nematic gels with partial degree of order

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Keywords: Active nematics, continuum mechanics, relaxation dynamics, spontaneous flow.

In this talk, we show how the theory of nematic elastomers can be a successful modeling paradigm for other, only distantly related, materials. The key idea is to decouple macroscopic and microscopic degrees of freedom, using a deformation gradient decomposition. While the observed deformations are macroscopic, microscopic degrees of freedom are incorporated in a coarse-grained manner by introducing material reorganization and relaxation. Specifically, when relaxation times are much faster than deformation times, one recovers the theory of nematic liquid crystals (Ericksen-Leslie). However, when these times are comparable, the theory captures polymer dynamics and viscoelastic behavior.

Furthermore, this theory also provides a natural and thermodynamically consistent framework for modeling active nematic gels [1]. Unlike standard theories, activity is not introduced as an additional term in the stress tensor, but rather as an external remodeling force that competes with the passive relaxation dynamics and drives the system out of equilibrium. The theory naturally describes the interplay of viscoelastic effects, defect dynamics, and self-ordering, which are characteristic of biologically active materials [2]. In a simple one-dimensional channel geometry, we show that even in the isotropic phase, the interaction between flow-induced local nematic order and activity leads to a spontaneous flow of particles.

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Orientational ordering of active nematics confined to a 2D nanoscopic ring-shaped cavity

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Keywords: Active nematics, confinement effect, molecular dynamics

We performed molecular dynamics simulations of model nonchiral and chiral active nematics confined to a two-dimensional nanoscopic ring-shaped region under both radial and tangential anchoring boundary conditions. These active nematics are composed of elongated particles which interact with each other through isotropic Lennard-Jones and anisotropic Maier-Saupe-like potentials. In addition, nonchiral particle's terminal appendage emits a jet of some substance generated by a certain internal chemical reaction, whereas chiral particles have an analogous lateral one. As a result, nonchiral particles are exposed to an additional reactive self-propelled force directed along their long axes, and chiral particles are exposed to both the reactive self-propelled force and torque that provides both an additional translational movement of particles and a self-rotation with respect to their geometric centers. The nonchiral active nematics presents an orientational order similar to that formed by the passive (without the self-propelled force) ones within the same ring-shaped region. In contrast, the chiral nematics exhibits significantly different orientational order from those observed by passive ones. In addition, when the chirality of active nematic particles is sufficiently strong, the orientational order within the ring-shaped region undergoes substantial time oscillations.

Out-of-Equilibrium GENERIC framework predicts Active Lyotropic Liquid Crystals

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Keywords: Activity, Lyotropic, Out-of-equilibrium, Simulations, Hydrodynamics

Controlling active lyotropic Liquid Crystal (LC) experiments, typically an active nematic coexisting with an isotropic fluid and molecular motors providing activity, remains a challenge due to unclear relationships between their component concentrations. This prompts questions about the general conditions transforming their chaotic dynamics into coherent motion. Consequently, continuum theory and simulations emerge as invaluable tools to predict and guide such experiments.

Here, we utilize the out-of-equilibrium GENERIC framework [1] to derive a thermodynamically consistent mathematical model for lyotropic LCs, treating time-evolution equations as the sum of energetic and entropic contributions. By doing this, we couple the momentum and energy balances with the concentration dependency as well as the liquid crystalline ordering. Next, we employ an upwind lattice Boltzmann hybrid scheme [2] to solve the resulting equations. We showcase three examples: 1) A study of a binary mixture in 2D at equilibrium, resembling chromonic LC data with +/- ½ topological defects [3]. 2) The introduction of hydrodynamics by incorporating a velocity parabolic profile and tracking the shape transition of an axial LC droplet immersed in an isotropic environment. 3) The addition of biochemical activity, resulting in turbulent simulations that flow naturally, akin to microtubule or actin realizations [4].

In short, this work addresses the challenge of obtaining reliable lyotropic LC simulations by leveraging cutting-edge computational and theoretical approaches. Our findings demonstrate the predictability of experimental data using the proposed GENERIC set of equations and these numerical techniques.

Acknowledgements: This work was partially funded by the Chicago Materials Research Center at the University of Chicago under NSF award number DMR-2011854.

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Simulation insights into mesophase formation using dissipative particle dynamics

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Keywords: dissipative particle dynamics, simulation, ferroelectric nematic

Molecular dynamics has proven to be a useful tool for explaining some of the fundamental aspects of liquid crystal phase behaviour. However, for complex systems, the required system sizes and time scales are often too demanding for atomistic models; therefore, coarse-grained models can be a useful for studying such systems. In this work we choose to use dissipative particle dynamics (DPD), which is a coarse-grained modelling approach in which multiple atoms are represented as 'beads'. The interactions between beads can be tuned to reproduce the effects of specific molecular interactions (e.g., dipole–dipole correlation).

We show that, using our relatively simple model, we can reproduce nematic and smectic phases, and mesophase transitions which result of from cooling. Most interestingly we use our model to represent the ferroelectric nematic phase, which has been poorly understood since its experimental discovery just a few years ago [1]. Previous MD simulations have struggled with the formation of the ferroelectric nematic phases due to significant energy barriers associated with alignment. In this work, we show that our liquid crystal phases can be generated either via pre-alignment, or by cooling from the isotropic phase.

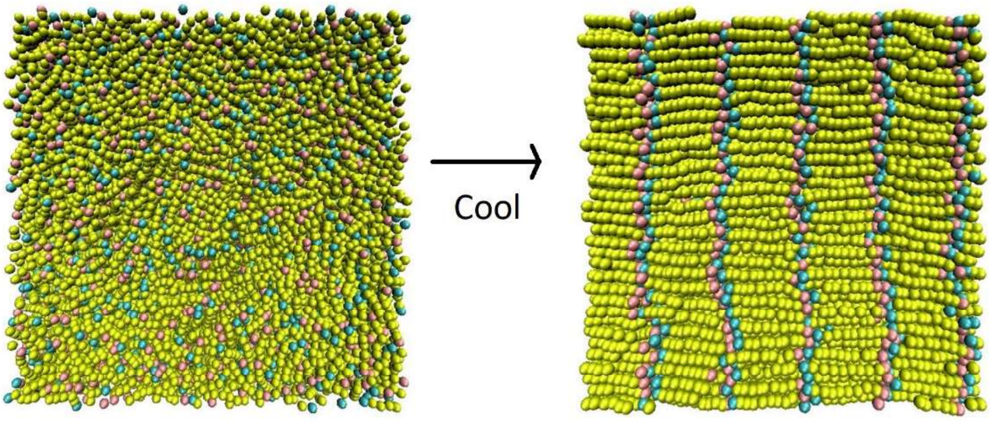

Figure 1: Transiton from an isotropic phase to a smectic A phase upon cooling. Terminating beads in the molecules are shown in pink and blue, while the middle of the molecule is shown in yellow.

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Theoretical approaches of optomechanical interactions between light and topological solitons

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Keywords: nonlinear optics, solitons, optomechanics.

In this contribution, I will present the theoretical and numerical advances we achieved that allowed us to recently model the interaction and co-assembly of optical and topological solitons in thin layers of cholesteric [1]. More specifically, we found that a delicate balance between the local transfer of momentum between light and matter and the nonlocal orientational elasticity of the liquid-crystal phase yield complex solitonic tractor beam behavior and self-patterning phenomena. I will show how a combination of free energy minimization techniques, beam propagation [2] and ray-tracing [3] simulations can be exploited to calculate the conservative and nonconservative components of the force that light exerts on a topological soliton, and will also provide a perspective on dissipative transport and out-of-equilibrium phenonema in liquid crystals.

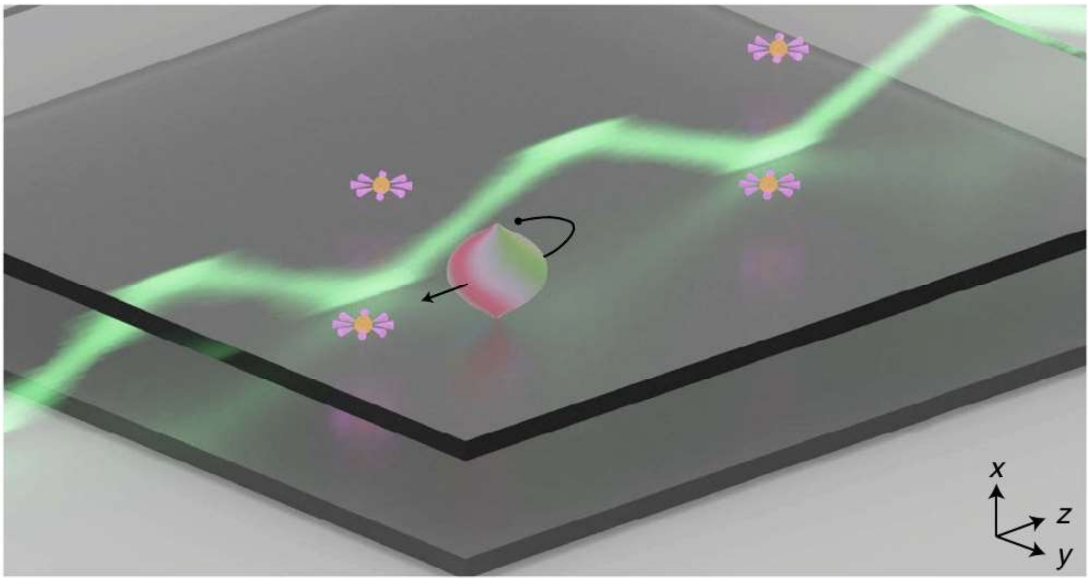

Figure 1: Schematic view of a toron (a simple example of point-like topological soliton) being guided by a bouncing optical soliton (in green) towards an equilibrium point.

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F2

Phases, structure, and ordering

Electric field effects on N–Sm-A–Sm-C phase transitions

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Keywords: Smectic liquid crystals, Phase transitions, Electric field, Phase diagram, Electroclinic effect

The effects of external fields on molecular ordering in liquid crystalline systems are an active research field [1] with major implications for developing new electro-optical devices [2]. In particular, the interplay of geometric anisotropy and different functional groups leads to anisotropic electromagnetic responses in thermotropic compounds [3]. The system's molecular orientation depends on both the compound's dielectric anisotropy and the orientation of the applied external field, which in turn modifies the order parameters and liquid crystalline sequence phases. For example, an external field can give rise to ordered phases well above the nematic-isotropic and smectic-isotropic bulk transition temperatures [4]. Moreover, birefringence measurements close to the nematic–smectic-A transition temperature have shown that strong electric fields suppress the nematic fluctuations in systems with a positive dielectric anisotropy, causing a crossover from first to second order phase transition. In this context, the present study is devoted to the investigation of phase transitions of a liquid crystalline system formed by rod-shaped molecules that have a small transverse dipole moment is analyzed in the presence of an external electric field normal to the smectic layers. The approach focuses on the phase transition diagram displaying the N–Sm–A-Sm-C phases, when both negative and positive dielectric anisotropies are considered. The analysis is carried out within the framework of an extended mean field theory, which shows the emergence of a reentrant Sm-C phase in the strong field regime, accompanied by a suppression of the translational ordering of the Sm-A phase, in the case of a negative anisotropy. A different scenario is observed in the case of positive anisotropy, as the electric field tends to suppress the Sm-C phase because the molecular alignment is driven by the field along its direction. In this case, the emergence of a residual nematic phase is also observed, which replaces the isotropic phase and is characterized by a low-value orientational order parameter.

Acknowledgements: This work was partially supported by Alagoas Research Foundation (FAPEAL), Brazil, the National Council for Scientific and Technological Development, Brazil (CNPq - 465259/2014-6), the Coordination for the Improvement of Higher Education Personnel (CAPES), Brazil, the National Institute of Science and Technology Complex Fluids (INCT-FCx), and the São Paulo Research Foundation, Brazil (FAPESP - 2014/50983-3). I. N. de Oliveira and Maria S. S. Pereira thank FAPEAL for the financial support (Grant No. E: 60030.0000002288/2022 and E: 60030.0000001635/2022).

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Geometric Modeling for the Isotropic-Smectic A Phase Transition

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Keywords: Smectic A, phase transition, energy landscape, free energy, Landau-de Gennes.

Liquid Crystals (LCs) present orientational and positional order that can be seen in synthetic and biological settings. This order is maintained until some parameter is changed, inducing a phase transition. Among these transitions a special sequence has been observed in which priority is given to the direct isotropic to smectic A (I-SmA) transition [1]. The synthesis and formation of LCs exhibiting this transition follow equilibrium self-assembly processes mainly driven by temperature and concentration [2]. The Landau-de Gennes (LdG) model is used to describe this type of transition by correlating the free energy of the system with orientational and positional order [3]. The phase transition kinetics seen in these models depends on stable, metastable, and unstable critical points on the energy landscape as seen in previous work [4]. Here, we take the findings on the self-assembly process, extend it to the self-organization scheme and present new soft matter methods to study the I-SmA phase transition. These methods integrate thermodynamic stability, index polynomial conservation, and geometric description to detect and describe stable and unstable phases. The characterization of the I-SmA energy landscape involves a two order parameter LdG model and three curve families: (I) polynomial index theorem, level-set curves, and steepest descent to describe the critical points and phase diagram; (II) lines of curvature and geodesics which are connected to the surface principal curvatures; and (III) the Casorati curvature and shape coefficient to assign simple shapes (e.g. sphere, cylinder, saddle) to the local surface geometry. In addition, the manifestation of these processes by nucleation and growth and spinodal transformation are studied by decomposing the index of the free energy polynomial into the contributions of the critical points at different quenching regimes (i.e. changes in temperature). Validation has been carried out using experimental data of an extensively studied compound that shows I-SmA behavior (12-cyanobyphenil) [5]. Consistent results were obtained for the phase diagram. Consequently, the three families showed the presence of nematic and plastic crystal phases that contribute to the phase transition behaviour. A lines of curvature network and geodesic lines demarked critical points trajectories as the quenching regime was changing. These highlighted energetic pathways that follow the phase transition. Finally, the shape coefficient and Casorati curvature showed the stability of the phases for the different quenching regimes.

Acknowledgements: DUZC thanks Consejo Nacional de Humanidades, Ciencia y Tecnología (853563), and McGill Engineering Doctoral Award for financial support.

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Molecular Simulations of Columnar Ordering in Triphenoxazoles - A New Class of Fluorescent Discotic Liquid Crystals

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Keywords: columnar phase, atomistic simulations, charge transport

Atomistic simulations are becoming a powerful tool for understanding molecular order in complex liquid crystalline phases.[1-3] Such simulations are able to rationalize how changes in molecular structure control the close packing of molecules, and how preferred molecular interactions can stabilize (or destablize) liquid crystal mesophases.

We perform atomistic simulations of representative mesogens from a class of newly synthesized fluorescent discotic liquid crystals. We demonstrate the spontaneous emergence of the columnar ordering, when cooled from the isotropic phase in simulations that extend into the µs regime. We characterise the columnar order and and its growth across the phase transition.

Our simulations show the formation of molecular stacks in the pretransition region and suggest that the transition into the columnar phase is achieved by the coalignment of these stacks. We analyse the structure of the columnar phase as well as the local arrangements of the molecules within the columns and discuss their implications for potential applications of this exciting class of compounds.

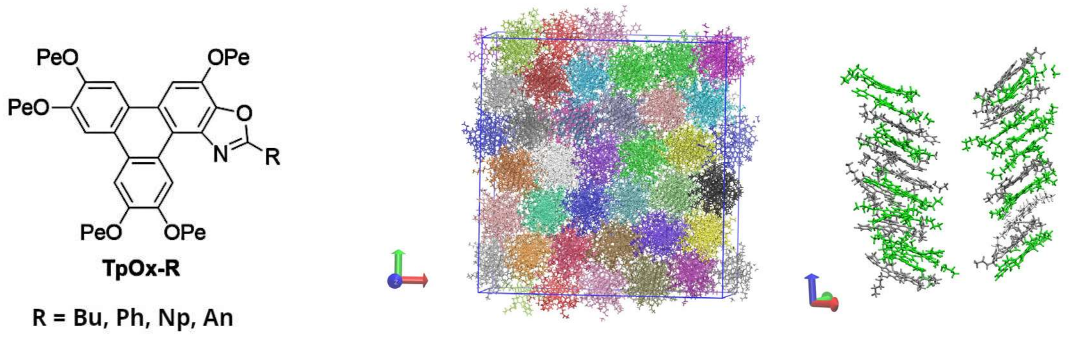

Figure 1: Left, chemical structures of the TpOx series; middle, simulation snapshot showing the ordering of columns in the columnar phase of TpOx-Ph; right, tilting of molecular cores in neighbouring columns in the columnar phase of TpOx-Ph.

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Reformulation of Elasticity Theory for Lipid Membranes, with Implications for Self-Assembled Microstructures

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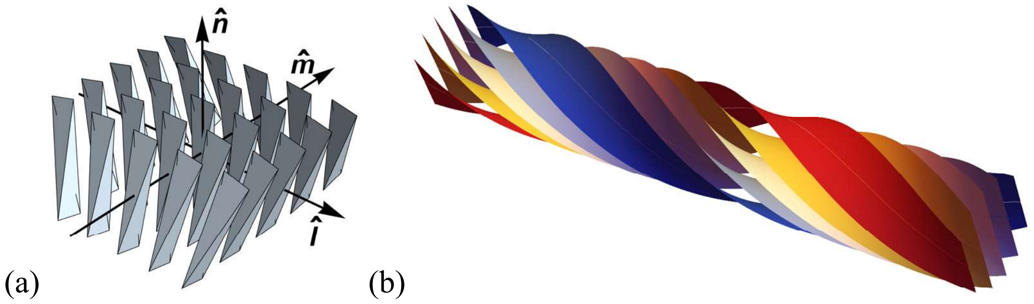
Keywords: Lipid membrane, Helfrich free energy, spontaneous curvature, octupolar order, self-assembly, tubule

The elasticity of lipid membranes is generally modeled using the Helfrich free energy, which is expressed in terms of the mean and Gaussian curvatures of the membrane. Here, we suggest a mathematical reformulation of the theory, which writes the free energy as the sum of squares of two modes. These two modes represent the sum and difference of principal curvatures, and are analogous to the splay and Δ deformation modes of nematic liquid crystals [1,2,3]. This reformulation shows how molecular shape and ordering can induce curved microstructures of lipid membranes. Polar order across the membrane leads to a favored sum of principal curvatures, as has long been recognized by the spontaneous curvature term in Helfrich theory. Likewise, octupolar order within the membrane leads to a favored difference of principal curvatures. We discuss how these mechanisms can explain experimental observations of the self-assembly of tubules, helical ribbons, and other lipid microstructures.



(a) (b)

Figure 1: (a) Octupolar order coupling with Δ deformation of director field [3].
(b) Self-assembled nanofilament, which may be induced by octupolar order [2].

Acknowledgements: This research was supported by grant number 2022197 from the US-Israel Binational Science Foundation (BSF), Jerusalem, Israel.

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Temperature reconfigurable skyrmionic solitons in cholesteric liquid crystals

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Solitons, topology, torons, cholesteric fingers, pitch

Chiral nematic liquid crystals (CNLC) possess a characteristic helical structure in which the liquid crystal director **n** continuously rotates around a helical axis at a constant rate. Pitch, *p*, is defined as the distance over which **n** rotates by an angle of 2π. The CNLC helical structure can be deformed in a number of ways, for example by confining the liquid crystal between surfaces with homeotropic anchoring or by applying external electric or magnetic field, to give rise to numerous topological solitons. Torons are topological solitons that cannot be continuously deformed into a topologically trivial uniform field[1]. In this study, torons are generated using a CNLC, 4-[(S,S)-2,3-epoxyhexyloxy]-phenyl-4-(decyloxy)-benzoate (W46), which is subjected to homeotropic anchoring and cooled down from isotropic temperature at varying cooling rates. The choice of the CNLC for this study is important because it displays a unique property where the pitch of the liquid crystal is strongly dependent on the temperature, displaying an inverse relation with it. It is observed that upon decreasing the pitch, torons act as seeds from which cholesteric fingers grow, and when the pitch is increased, the cholesteric fingers shrink back to form torons[2]. During the heating-cooling loops, the morphology of torons is severely deformed, yet the process is reversible and the torons are very well topologically protected (fig.1). It is also observed that adjusting cooling rates influences toron density: faster cooling results in higher toron density, while slower cooling leads to a lower toron number density. Toron properties have been observed to be influenced by other factors, such as cell gap and surface anchoring strength. Experiments investigating the effects on toron packing and size have been conducted, showing promising results. Although additional experiments are needed, these findings offer valuable insights into torons and their potential applications in various fields, including physics, chemistry and biology, where topological solitons are already receiving increasing attention.

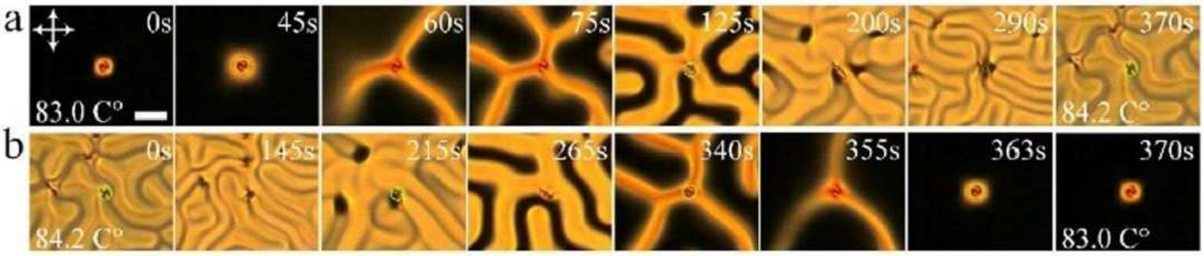

Figure 1: Time series of polarizing photographs showing reversible transformation between torons and cholesteric fingers (a) for decreasing pitch and (b) increasing pitch. Scale 20 µm.

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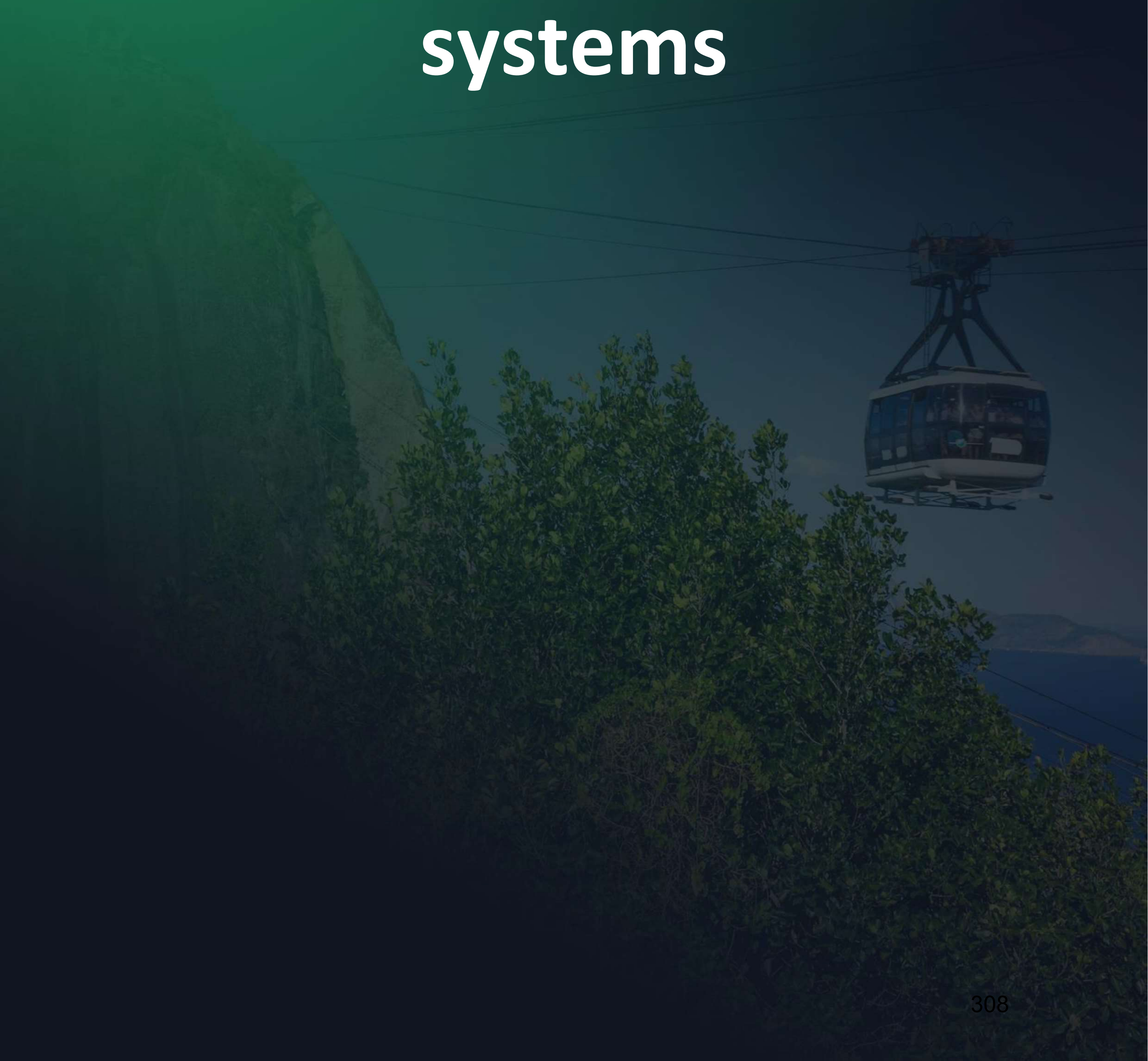
F3

Frustrated phases and complex systems



Anisotropy of Crystal Growth in Blue Phase I Transitioned from Uniformly Oriented Cholesteric Phase

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Keywords: blue phase, nucleation, crystal growth, orientation control

Cholesteric blue phases (BPs) are chiral liquid crystalline (LC) states in which directors self-organize into a double twisted cylindrical structure. They possess unique properties such as optical isotropy, reflection of circularly polarized light at visible wavelengths, and fast electric field response, making them promise for applications in displays, phase modulators, biosensors, and tunable lasers. Initially considered to be materials free from the rubbing process due to their optical isotropy, recent studies have highlighted the importance of the lattice orientation control in enhancing device performance. Although BPs are LC phase, they form quasi-crystalline structures with molecular orientations on the order of several hundred nanometers, resulting in phase transition behavior similar to that of crystalline solids. This complicates the BP orientation mechanism and makes orientation control difficult. Therefore, understanding the phase transition and crystal growth is crucial for improving the orientation of BPs. The behavior of the BPs phase transition is significantly influenced by the preceding phase state: in the Iso-BPI phase transition, BPI exhibits facets and crystal morphology similar to a crystalline solid [1]; in the BPII-BPI phase transition, the transition is martensitic [2]. Thus, the phase transition in BPs represents an interesting phenomenon, not only from the technical aspect of orientation control, but also from the theoretical perspective of analogy with crystalline solids.

In this study, we focused on the phenomenon where BPI crystals exhibit a square shape upon the phase transition from the uniformly oriented Ch phase to the BPI phase. BPLC was filled in a rubbing cell with a thickness of 5 µm, and the temperature was slowly raised at a rate of 0.01 °C/min from the Ch phase to transition to the BPI phase. The square shape of the BPI crystals, which was observed in three types of BPLC materials with different elastic constants, had its diagonal direction corresponding to the [010] crystal axis. This indicates an anisotropy in crystal growth rate, with the [010] axis direction growing faster than the [011] axis direction. Moreover, the in-plane crystal orientation was correlated with the easy axis, showing a tendency for the [011] axis to coincide with the easy axis, though the easy axis had little effect on the crystal growth rate. Furthermore, it was found that scratches on the substrate surface promote nucleation. Utilizing this behavior, we demonstrated that the nucleation position and density can be controlled by intentionally disturbing the Ch orientation through locally changing the easy axis using photoalignment.

Acknowledgements: We thank DIC Co. for providing the alignment agent. This work was partly supported by MEXT KAKENHI (JP21K18722, JP23H02038) and a Grant-in-Aid for JSPS Fellows (23KJ1507).

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Controlling flow patterns and topology in active emulsions

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Keywords: Active Liquid Crystals, Topological confinement, Numerical simulations.

Active emulsions and liquid crystalline shells are intriguing and experimentally realizable types of topological matter [1,2]. Here we numerically study the morphology and spatiotemporal dynamics of a double emulsion, where one or two passive small droplets are embedded in a larger active droplet [3]. We find that activity introduces a variety of rich and nontrivial nonequilibrium states. First, a double emulsion with a single active droplet becomes self-motile, and there is a transition between translational and rotational motion (Fig. 1a): both regimes remain defect-free, hence topologically trivial. Second, a pair of particles nucleate one or more disclination loops, with conformational dynamics resembling a rotor or chaotic oscillator, accessed by tuning activity. In the first state a single, topologically charged, disclination loop powers the rotation (Fig. 1b). In the latter state, this disclination stretches and writhes in 3D, continuously undergoing recombination to yield an example of an active living polymer (Fig. 1c). Finally, we consider the effect of passive chirality on the dynamics of the active liquid crystals. Multiple emulsions provide a pathway to stabilize flows and topology patterns in active matter in a controllable way, as opposed to bulk systems that typically yield active turbulence.

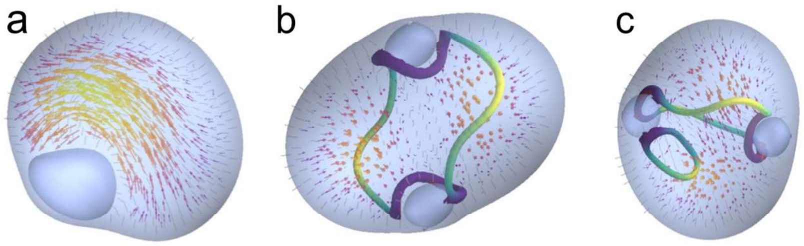

Figure 1: Multi-core active emulsions. (a) An extensile active liquid crystal (headless rods) is confined in a double emulsion and generates a self-sustained flow (colored arrows) inducing the rotation of the inner isotropic core. (b-c) Two-core emulsions consists of an active nematic droplet encapsulating two passive isotropic droplets, therefore stabilizing a disclination loop. Activity can induce the rotation of the defect line (panel b) or lead to the chaotic a chaotic behavior including the nucleation of additional defect lines (panel c).

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X-ray detected consequence of ultra-small curvature radius of smectic layers: dilation and chevron formation

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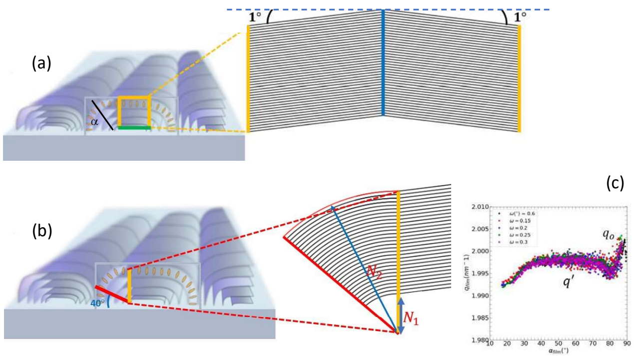
Keywords: smectic, elasticity, topological defects, distortion.

The smectic phase bridges the study of broken orientational symmetry *à la* nematic order, the statistical mechanics of membranes, and the long range periodic order of crystals. As such, it can be probed optically, mechanically, and through X-ray diffraction. From a theoretical perspective, it provides an arena to systematically study the effects of nonlinear elasticity via fluctuations [1] topological defects (where the distortions can be large) [2], and, as we will demonstrate here, even in complexions arising from antagonistic boundary conditions. By studying regions of high layer curvature via Grazing Incidence Small Angle X-ray Scattering (GISAXS) we have measured, with spatial resolution, the layer spacing and find that it is accurately described by the nonlinear response of bent layers under antagonistic anchoring.



Between planar unidirectional and homeotropic anchoring, smectic layers bend into arrays of flattened hemicylinders (fig.1) [3]. We show that for a film thickness 180 nm, the flattened hemicylinders center is formed by slightly tilted layers with a chevron (fig.1a in blue). The respective intralayer spacings of rotating and central tilted layers are different as shown by the high-resolution X-ray measurements resolved by the angle of the layer normal (fig.1c). A junction between the two kinds of smectic layers is thus induced (fig.1b in yellow). We minimized the non-linear elastic energy of one given hemicylinder to show that a dilation is induced in the rotating layers to relieve the large bending energy. We calculated the exact dilation for each rotating layer that depends on the inverse square of the smectic layer curvature radius. Dilation as high as 1% are reached for the smectic layers closest to the curvature center. Calculated and measured average dilations perfectly agree (see fig.1c where the average wave-vector transfer, q = 2π/d, d being the average intra-layer spacing, is measured as a function of α, the layer normal orientation – q' for rotating layers (α < 85°) is smaller than q_o for central layers (α = 89°)). We also perfectly predict the measured 1° tilt of the central layers. This dilation is a direct consequence of the smectic non-linear elasticity. It may occur in all systems of small curvature radius, like, for example in focal conics in the areas closest to the topological ellipse.

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F4

Dynamics and pattern formation

Active and driven nematic topological defects

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Nematic fluids are characterised by internal orientational order, which upon tuning or frustration, can exhibit topological defects. In active or driven nematics, topological defects emerge as dynamic objects that exhibit complex regular or irregular dynamics. Here, we give an overview of dynamic structures of topological defects in three-dimensional active and driven nematics. Specifically, we show defect profiles in three-dimensional active turbulence, under confinement and in bulk. We discuss the nature of three-dimensional defect loops and their changing local director structure. We show refinement and coarsening upon changing the activity and present continuous generation of topological defects in a passively driven nematic.

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Controlling Active Nematic Topological Chaos Through Defect Pinning on Sharp Boundary Features

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Keywords: topological defects, fluid mixing, ordered flows, braid theory

In active nematic liquid crystals, topological defects drive chaotic flows in the bulk. Confined geometries with uniform curvature have been shown to produce ordered defect motion and flows[1,2]. However, little is known about ordered defect motion enabled by boundaries with varying curvature. To explore how varying curvature can control the active steady state, we simulate an active nematic system using active Beris-Edwards nematodynamics with curved boundary walls. In particular, we investigate the effects of varying bulk topological charge via pinning defects on boundary features. We show that locally convex and concave boundary features have defect pinning effects on positive and negative topological charge respectively, and demonstrate a scheme to tune the strength of defect pinning, expanding the possibilities of ordered states [Figure 1(left)]. Using tools from braid theory, we characterize the trajectories and topological entropy associated with fluid mixing resulting from ordered defect motion [Figure 2(center, right)] and show that active nematics can generate maximally mixing braids in their confining geometries. Our findings suggest routes to controllable bulk active flows utilizing boundary features.

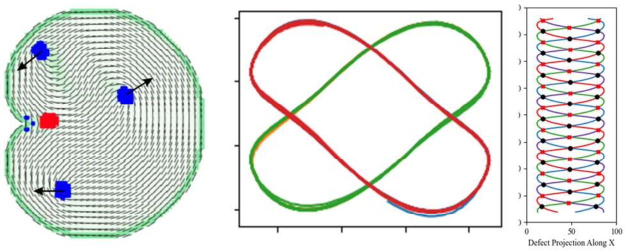

Figure 1:
Left: -1/2 (red) topological defect pinned at the cusp of a cardioid, thus requiring three +1/2 topological defects in the bulk. Center: The trajectories of four +1/2 topological defects shown from above in an ordered flow. Right: The trajectories of the center panel shown as a projection along an axis over time.

Acknowledgments: This material is based upon work supported by the National Science Foundation under Grant No. DMR-2225543

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Emergence and transitions of disordered branching patterns in confined chiral nematic liquid crystals

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Keywords: Chiral liquid crystal, Branching process, labyrinthine pattern, self-organization

Spatial branching processes are ubiquitous in nature, but the mechanisms that drive their growth can vary significantly from one system to another. In soft matter physics, chiral nematic liquid crystals provide a controlled environment to study the emergence, growth, and transition of disordered branching patterns. A cholesteric phase can nucleate in a chiral nematic liquid crystal by applying appropriate forcing (thermal, electrical, and magnetic). This phase self-organizes into an extended branching pattern, with branching events occurring when the rounded tips of cholesteric fingers become unstable and split into two new cholesteric tips. The origin of this interfacial instability and the mechanisms that drive the large-scale spatial organization of these cholesteric patterns are still unclear. In this talk, we will study and investigate the spatial and temporal organization of thermally driven branching patterns in chiral nematic liquid crystal cells and describe the observations through a mean-field model. The findings indicate that chirality plays a crucial role in the formation of fingers, regulates their interactions, and controls the process of tip-splitting. We will demonstrate that the complex dynamics of the cholesteric pattern behave as a probabilistic process of branching and inhibition of chiral tips, which drives the large-scale topological organization. The theoretical findings align well with the experimental observations.

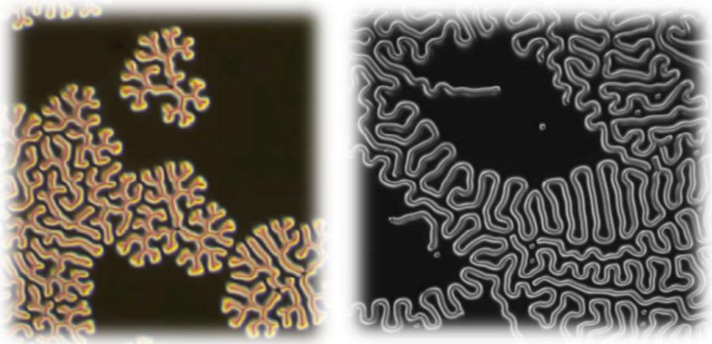

Figure 1: Disordered branching patterns in confined chiral nematic liquid crystals.

Acknowledgements: financial support of ANID-Millennium Science Initiative Program-ICN17_012 (MIRO) and FONDECYT project 1210353.

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Morphogenesis of a cholesteric liquid crystalline droplet with structure rotation under temperature gradient

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Keywords: cholesteric liquid crystal, non-equilibrium, temperature gradient

Morphologies of living organisms are formed via ordering and disordering with various size scales, as seen in segmentation and differentiation of eggs or metamorphosis of insects. Such hierarchical structure formations can be observed also in liquid crystalline systems.

In this study we prepared a cylindrical droplet, using a cholesteric (Ch) liquid crystal (Fig.1(p)). Applying a constant temperature gradient and cooling the droplet from the isotropic (I) state, we obtained the Ch droplet via the coexistence state (I+Ch) as shown in the polarizing microscope (POM) images of Fig.1(a)–(f). In this 1st cooling process the director field was gradually formed in the droplet, and the director rotation was observed when the field was not circular symmetric. After that, by performing specific heating and cooling operations, we obtained the Ch droplet with a different structure from that before the operations (Fig.1 (f) and (o)). In these 1st heating and 2nd cooling processes, the director rotation was also observed as well as in the 1st cooling, while the rotational direction depended on the temperature.

Moreover, microscope observation without polarizers revealed that defect loops existed in the droplet and the recombination of them occurred at the end of the 1st heating process. This topological change is considered to be the main reason of the structural change (Fig.1 (f) and (o)) induced by the heating and cooling operations.

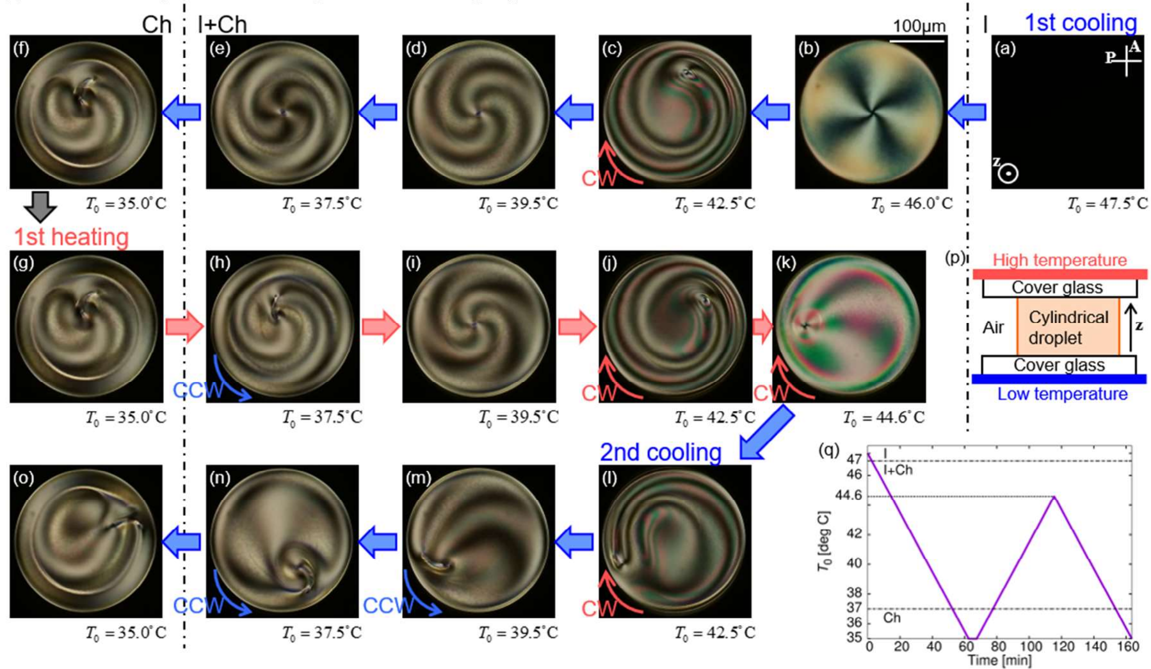

Figure 1: Structural formation of a Ch droplet. (a)-(o) show polarizing microscope (POM) images at each T_0, defined as the temperature at the droplet center. The schematic image of the experimental system is shown in (p), and the T_0 chart is in (q). Clockwise (CW) rotation was observed in (c), (j), (k) and (l), while counterclockwise (CCW) was in (h), (m) and (n).

Nonlinear Waves Propagation in a Bistable Optical Chain with Nonreciprocal Coupling

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Keywords: Nonlinear Optics, Nonequilibrium Physics, Nonreciprocal Systems

Fronts are nonlinear waves that appear in several everyday physical contexts. The propagation of fronts, such as fires, weather fronts, and the spread of diseases, has been the subject of special attention. An example from daily life is domino waves, which propagate equally towards the left or right flank owing to the reciprocal coupling between each piece, where both elements of the same system interact equally independently of the direction of interaction. However, the effect of nonreciprocal coupling on the front propagation where the energy emitter and receiver are not exchangeable is not well understood. Based on an experiment on a bistable optical chain forced by nonreciprocal optical feedback, we can study the propagation of fronts. A spatial light modulator and high-resolution optical feedback allow us to control the initial conditions and change the coupling between the chain elements shifting the optical feedback in α. The spatiotemporal evolution and front speeds were characterized, showing the maximum front speed for large nonreciprocal couplings. A theoretical model is derived for interacting optical elements in a liquid crystal light valve with nonreciprocal optical feedback. The numerical simulations agree with the experimental observations.

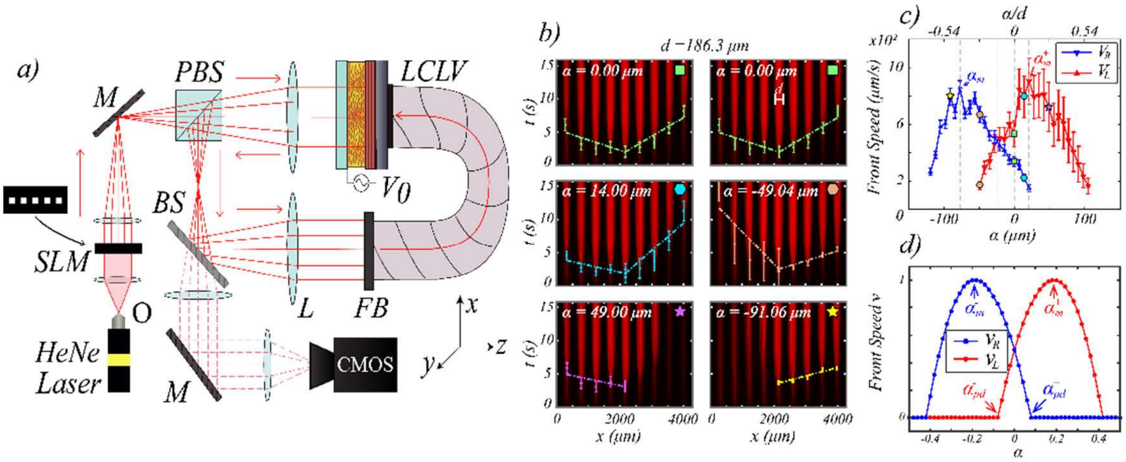

Figure 1: a) Schematical representation of experimental setup. b) Experimental spatiotemporal diagrams of front propagation for different α. Average propagation velocity for a sweep of α: c) Experimental results, d) numerical simulations.

Acknowledgements: This work was funded by ANID-Millennium Science Initiative Program-ICN17 012 and Fondecyt project 1210353.

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Turbulent labyrinthine patterns in liquid crystal light valve with optical feedback

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Keywords: Nonlinear Optics, Pattern Formation, Nonequilibrium Physics, Turbulence, Chaos.

Systems with energy injection and dissipation self-organize by forming patterns of stripes, hexagons, squares, and superlattices at the onset of spatial instabilities. Increasing the disproportion between injection and dissipation of energy generates the emergence of disordered patterns with complex spatiotemporal behaviors. We investigate the turbulent dynamics of labyrinthine patterns far from the primary spatial instabilities in a liquid crystal light valve (LCLV) with an optical feedback experiment [1]. Using statistical tools [2,3], we reveal the turbulent and intermittent nature of the intensity field. We reveal phase and defects turbulence characterized by power-law spectra with exponents -2 and -3, respectively. The pattern orientation field also presents a power law spectrum with exponent -2. The largest Lyapunov exponent is determined experimentally and shows that the observed dynamics is chaotic. We provide a phenomenological model to capture the experimental observations.

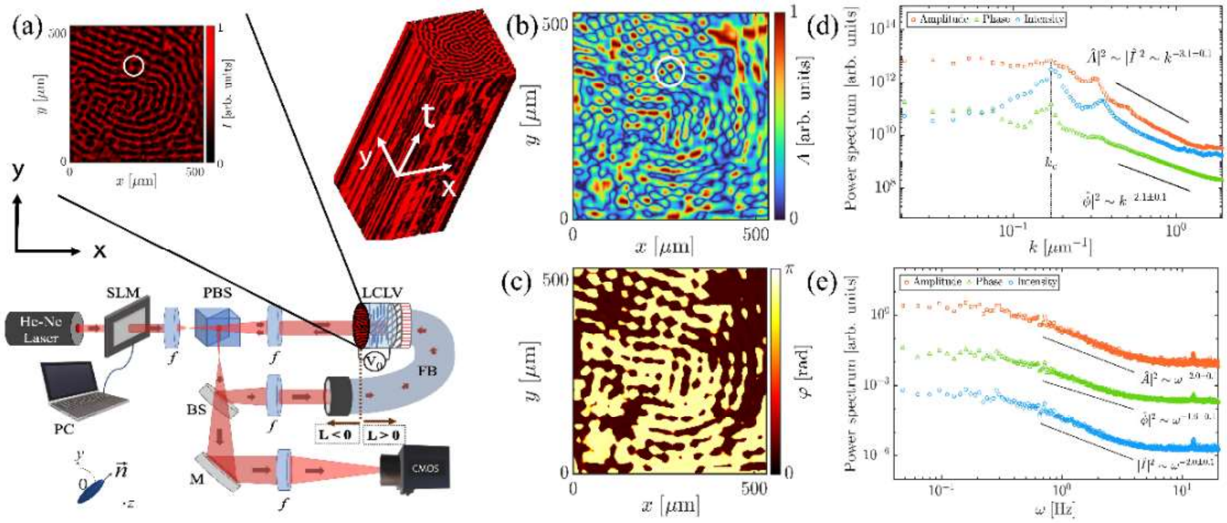

Figure 1: (a) Schematic representation of a liquid crystal light valve with optical feedback and instantaneous intensity field and the corresponding amplitude (b) and phase (c). The white rings illustrate the position of a defect in the intensity and amplitude fields. Spatial (d) and temporal (e) power spectra of intensity, phase, and amplitude.

Acknowledgements: This work was funded by ANID-Millennium Science Initiative Program-ICN17 012 and Fondecyt project 1210353.

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Vortex triplet dynamics in a nematic liquid crystal cell.

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Keywords: Nematic, vortices, topological charge, hysteresis.

By applying an oscillatory electric field onto an homeotropic nematic liquid crystal cell it is possible to induce vortices, which are particle-type defects with topological charge. The dynamics of the vortices is such that topological charge of the system is conserved[1]. Using a magnetic ring and a sinusoidal voltage it is possible to induce a vortex triplet[2], characterized by a positively charged vortex close to the center of the ring, and two vortices op opposite charge each on either side of the central vortex. Recently we observed that increasing the intensity V_0 of the sinusoidal voltage results in a decreasing of the separation distance between the negative vortex and the central vortex. At a critical intensity V_u these two vortices annihilate, leaving only the positive vortex of the side. In this state, if the voltage intensity is decreased, the vortex pair reappears at an intensity V_d, with $V_d<V_u$. By considering the interaction of the vortices between each other and with the environment, and applying different approximations[1], it is possible to obtain a differential equation for the evolution of the distance between the negative and central vortex, which presents a similar hysteresis region. Simulations of the vortex triplet made from the amplitude equation of the system also show this transition and are therefore consistent with experimental observations.

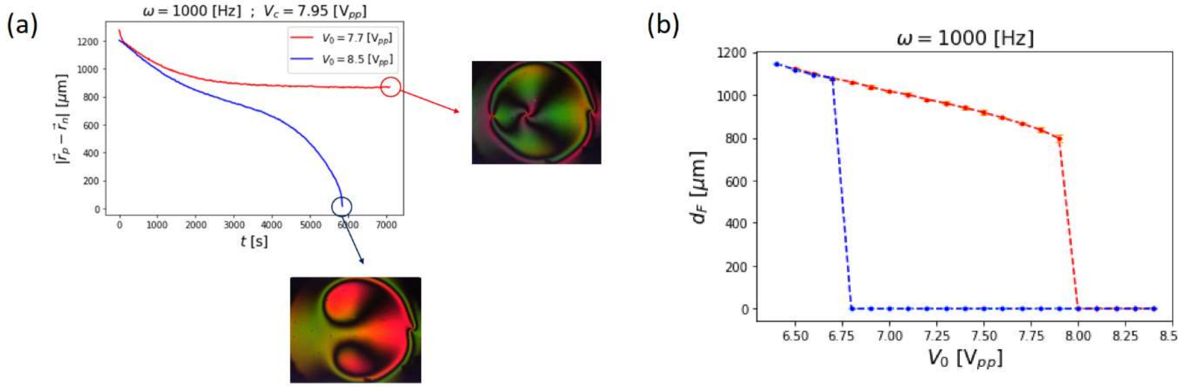

Figure 1: (a) Separation distance of vortices as a function of time for $V_0<V_u$ (red) and $V_0>V_u$ (blue), and snapshots of stationary state for each intensity. (b) Stationary separation distance of vortices as a function of intensity V_0 increasing (red dots) and decreasing (blue dots) this value. The hysteresis region is delimited by the values V_d=6.8 V_{pp} and V_d=7.9 V_{pp}.

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F5

Surfaces, confined systems, and alignment control

Explicit Q-tensor descriptions of Singularities around Colloidal Particles in Nematic Liquid Crystal

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Keywords: Colloids, boojums, Saturn ring

Describing defect structures in nematic liquid crystal colloids present an important but challenging task. In the small particle limit of the Landau-de Gennes model, it is possible to obtain explicit descriptions of the minimizing Q-tensor field and its singularities. For homeotropic anchoring and a single spherical particle, such a solution has been obtained in [1].

We will present several generalizations of this result in a variety of situations: we prove the presence of a Saturn ring defect also for ellipsoidal particles and determine the optimal orientation of the particle with respect to alignment at infinity, see [2] for a numerical investigation. We also investigate the structure of defect lines for two spherical particles. Depending on the particle distance, an additional line singularity between the particles forms, that may or may not be connected to the line encircling both particles, similar to the entangled hyperbolic defect configuration in [3]. Furthermore, we determine minimizers for different planar boundary conditions around a single spherical particle, showing that the defects consist of two boojums, situated at opposite poles of the particle as numerically explored in [4]. With our method, we are also able to compute explicitly the minimizer for conical anchoring boundary condition.

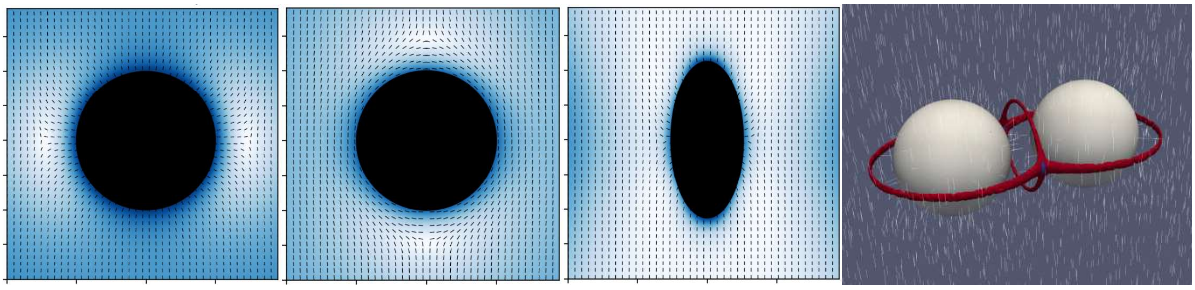

Figure 1: Director field around spherical and ellipsoidal particles obtained from explicit solutions with homeotropic or planar anchoring. On the three images on the left, color indicates the norm of the Q-tensor, on the right the region where the two leading eigenvalues are equal is shown.

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Kinetics of annealing of LC shells depending on the wall thickness

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Keywords: Liquid Crystal Shells, Annealing Kinetics, Wall Thickness, Topological Defects

In this study, we investigate the kinetics of annealing in liquid crystal (LC) shells depending on wall thickness. As it is known, most often, LC shells are asymmetric in shape due to density mismatch driving the inner isotropic droplet up or down within the LC, yielding antipodal points of minimum and maximum thickness within the shell [1, 2]. While exploring the production and stability of 5CB shells across a range of concentrations of polyvinyl alcohol (PVA) aqueous solutions, it was observed that the speed of shell relaxation was affected by their average wall thickness.

Examination through polarized optical microscopy (POM) images revealed that the thicker-walled shells exhibit shorter relaxation times compared to thinner-walled ones. For instance, in 0.25 wt. % PVA, 5CB shells with an average wall thickness of ~23.6 µm required not more than 3 minutes to anneal, whereas 5CB shells with an average wall thickness of ~10 µm needed around 13 minutes to acquire their final tangential alignment (Figure 1).

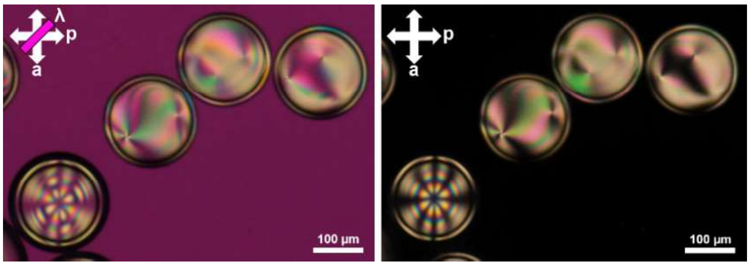

Figure 1: An example of transmission POM images of 5CB shells in 0.25 wt% PVA as inner and outer phases. The shell in the lower left corner with an average wall thickness of ~23.6 µm needed not more than 3 minutes to anneal and the rest shells with an average wall thickness of ~10 µm needed 13 minutes to anneal.

We attribute this phenomenon to the relationship between the LC shell's average wall thickness and the distribution of topological defects. Thinner-walled shells exhibit a more uniform thickness distribution, leading to prolonged persistence of topological defects around the spherical shell until they concentrate in the shell's thinner part. In contrast, thicker-walled shells, being even more asymmetric, acquire their final tangential alignment more rapidly.

This study emphasizes the role of wall thickness on the annealing kinetics of LC shells.

Acknowledgments: University of Luxembourg, Experimental Soft Matter Physics group

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Liquid Crystal Soft Interface Microfluidics

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Keywords: Nematics, microfluidics, interfaces, response

Nematic liquid crystals (LCs) are simple and promising alternatives in future sensor technologies that have been shown to be successful in detecting small to macro-sized analytes (ranging, e.g., from gaseous molecules to proteins).[1] However, attempts to date were mostly designed based on stagnant LC systems, which limit their use in automated, high-throughput analysis systems. We are currently studying a flow system where LCs are in contact with aqueous, soft interfaces to develop a platform that can provide a forward leap towards their integration into such systems. We used photolithography, wet-etching, and surface functionalization to fabricate glass microfluidic channels such that the two distinct fluid phases (aqueous phase and LC) flow in separated, predetermined paths, while maintaining an intact, stable LC-aqueous interface. We show that the LC-aqueous interface was intact up to 35 mbar of pressure difference across the interface, which was reduced with the presence of surfactants. Such stability allow independent manipulation of the flow rates and arrangements of the two phases in contact with each other. We observed a shear-induced alignment transition from weak to strong flow regime with the measured alignment of mesogens within ~10° to 90° relative to the surface normal, which was influenced by the shear induced by the neighboring aqueous phase. Beyond shear, we also show that the flow and configurations of LC-aqueous soft interfaces were responsive against surface and interfacial heterogeneities. We present the promising outcomes of our study that demonstrate a forward leap for the next-generation, analytical flow systems.

Acknowledgements: Funded by the European Union (ERC, LCFlow, 101039294).

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Photochemical Control of Optical Properties and Chiral Mesophases in Liquid Crystal-Core Electrospun Fibers

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Keywords: Electrospinning, fibers, chiral, photochemical, optics

Microscale confinement of liquid crystals produces a rich tapestry of mesophases that exist in a very particular set of parameters. In our work, we fabricate electrospun fibers that envelope a several-um-diameter thick liquid crystal core in a polymer sheath. First, we demonstrate the use of photochromic azobenzene-based surfactants embedded in the polymer sheath to change the surface properties of the liquid crystal core and induce a phase transition [1]. For a quantification of the surface effect, we calculate the interference colors of the fibers and explore the effect of thickness and birefringence both experimentally and theoretically using the dispersion of the liquid crystal material [2]. We then use UV light to photoisomerize the photochromic surfactants and induce a change in color. From this, the change in nematic order, which manifests as a change in birefringence, of the liquid crystal in the core is quantified. Finally, we add a chiral dopant to the nematic liquid crystal to induce a cholesteric phase. While the system properties continuously change with increasing temperature, the liquid crystal transitions through discretized chiral mesophases that are anchored by the surface. Using the photochromic surfactants in the polymer sheath to change the surface anchoring properties, we demonstrate photochemical control over these mesophase transitions.

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Macroscopic biaxial order in multilayer films of bent-core liquid crystals deposited by combined Langmuir-Blodgett/Langmuir-Schaefer technique

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Keywords: bent-core mesogens, Langmuir films, biaxiality, GIWAXS, neutron reflectivity

Bent-core mesogens (BCMs) are well-known for their unconventional mesophases characterized by complex supramolecular ordering often featuring biaxial and polar properties. In the nematic (N) phase their unique behavior is manifested in the formation of cybotactic groups[1,2], i.e. nano-sized biaxial clusters of stratified molecules. While this has attracted great interest for their potential in the quest for nematic biaxiality, experimental evidence has shown that spontaneously, i.e. without any external aligning action, biaxial order is only short-ranged and that the N phase is macroscopically uniaxial[3]. Nonetheless, the capability to finely control the orientation of the N director by means of proper anchoring conditions represents a critical issue in the experimental study of BCMs as well as in their use in electro-optical devices.

By combining a battery of complementary techniques including atomic force microscopy, neutron reflectivity and wide-angle grazing-incidence X-ray scattering, here we show that multilayer films of a bent-core nematic, deposited on silicon by a combined Langmuir-Blodgett and Langmuir-Schaefer approach, exhibit macroscopic in-plane ordering, with the long molecular axis tilted with respect to the sample surface and the short molecular axis aligned along the direction of the film compression, thus resulting in a macroscopic biaxial arrangement[4,5]. Hence, the described deposition technique represents an effective strategy to enhance the BCM natural tendency to biaxial ordering, forcing the mesogens to adopt a uniform organization over large areas and extending biaxial order from the nanoscale to the macroscopic scale. The results of our investigations demonstrate that the Langmuir-film technique is an effective way to study and control the complex anchoring properties of BCMs.

Acknowledgements: We acknowledge the ESRF and ALBA synchrotrons for the provision of beamtime

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F6

Artificial Intelligence applied in liquid crystal science

Determining liquid crystal properties with machine learning methods

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Keywords: Liquid Crystals, Machine Learning, Complexity-Entropy, Ordinal Networks

TMachine learning methods are becoming increasingly important for the development of materials science. In spite of this, the use of image analysis in the development of these systems is still recent and underexplored, especially in materials often studied via optical imaging techniques such as liquid crystals. Here we present two different approaches to characterize and make predictions of liquid crystal's physical parameters. The first approach [1] combines two physics-inspired image quantifiers (permutation entropy and statistical complexity) with machine learning techniques for extracting physical properties of nematic and cholesteric liquid crystals directly from their textures images. We demonstrate the usefulness and accuracy of our approach in a series of applications involving simulated and experimental textures, in which physical properties of these materials (namely: average order parameter, sample temperature, and cholesteric pitch length) are predicted with significant precision. The second approach [2] uses ordinal networks to map optical textures obtained from experimental samples of liquid crystals into complex networks and use this representation jointly with a simple statistical learning algorithm to investigate different physical properties of these materials. We demonstrate that the method is capable of identifying and classifying mesophase transitions, distinguishing among different doping concentrations used to induce chiral mesophases, and predicting sample temperatures with outstanding accuracy. The precision and scalability of our approach indicate it can be used to probe properties of different materials in situations involving large-scale datasets or real-time monitoring systems.

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Others

Analysis of the in vivo biological activity of novel synthetic angiotensin 1-7 peptides

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Keywords: Angiotensin 1-7 analogs, peptides, liquid crystals, biological activity, anxiety, nociception

Amino acids, peptides, and their derivatives are important molecules in mammalian organisms that activate or inhibit enzymes and receptors through covalent and non-covalent bonding forming complicated regulatory systems. Smaller linear peptides and amino acid molecular motifs are structural parts of mesogenic molecules designed for many liquid crystals (LCs) phases with specific properties depending on the applications in different fields. The heptapeptide angiotensin (Ang 1-7: Asp-Arg-Val-Tyr-Ile-His-Pro), acting on the Mas receptor, is a member of the balancing arm of the renin-angiotensin system (RAS), which regulates blood pressure and electrolyte homeostasis and modulates some key brain functions.

The present study is focused on synthesizing and characterizing the biological activity of some new structural analogs of the native peptide Ang 1-7. Solid-phase peptide synthesis—Fmoc-strategy—was used to create the new peptide analogs. Crude Ang 1-7 peptides were purified on RP-HPLC and molecular weights, electrochemical properties, and specific optical rotation angles were determined before testing in behavioral experiments. The biological activity of the synthesized peptides was evaluated using a battery of behavioral methods including the "open field" test for exploratory activity, the "elevated plus maze" test for anxiety-like activity, and the formalin test for acute and inflammatory pain in experimental ICR mice.

The new peptide analogs showed good solubility in saline and were suitable for intraperitoneal injection. The dose was chosen based on literature data for the precursor peptide and was administered once before the tests. Three of the peptide analogs decreased exploration and potentiated anxiety-like behavior in a novel environment. They inhibited acute nociception and significantly reduced subchronic inflammatory pain induced by a chemical irritant. One of the newly synthesized analogs showed no significant effects relative to controls and exhibited weaker effects compared to the precursor peptide.

These initial data encourage further analysis of the designed peptides, considering their selectivity to target receptors and potential implementation in the therapy of unbalanced RAS.

Acknowledgements: This work was financially supported by the Bulgarian National Scientific Fund project КП-06-Н71/9 of the Ministry of Education and Science, Bulgaria.

Synthesis, characterization and biological study of new renin-angiotensin molecules

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Keywords: Angiotensin analogs, peptides, liquid crystals, physicochemical characteristics, electrochemistry

The heptapeptide Angiotensin (Ang 1-7: Asp-Arg-Val-Tyr-Ile-His-Pro) is a vasodilating agent that is part of the renin-angiotensin system (RAS) and it is also an antagonist of the Mas receptor. It can be formed by cleavage of Ang I by neprilysin or from Ang II through Angiotensin Converting enzymes (ACEs). Amino acids and peptides play important roles in both living and non-living systems, allowing them to create molecular structures through covalent bonding and non-covalent interactions. In material chemistry, peptides play an important role in liquid crystals (LCs), particularly in the rapid formation of supramolecular hierarchical networks. The use of amino acids and peptides in LCs enables various inherent properties, such as side chain variety, chirality, directionality, reversibility, and stimuli-responsive complex molecular structures. The smaller molecular motifs of amino acids and linear peptides as structural components of mesogenic molecules resulted in several LC phases with features such as lyotropy and thermotropy, as well as applications in a variety of fields of biology and medicine.

Some new structural analogs of the native peptide Ang 1-7 analogs with conformationally constrained amino acids have been synthesized, characterized, and tested for biological activity. Some physicochemical characteristics of these biomolecules were also measured using different analytical techniques. Solid-phase peptide synthesis—Fmoc-strategy—was used to create the new peptide analogs. The crude Ang 1-7 peptides were purified on an RP-HPLC and the molecular weights were determined, using ES-MS, and also determining the specific angles of optical rotation. The electrochemical properties were also discussed and confirmed the fact that some transformation in amino acids skeleton changes the electrochemical behavior of the compound by altering the reactivity of the redox function group. Some new peptide analogs with conformationally constrained amino acids demonstrated a strong antinociceptive effect, excellent saline solubility, and efficacy after local application in soft tissues. The compounds were designed using the approach of increasing their aqueous solubility and/or affinity for the target receptor or enzyme.

Acknowledgements: This work was financially supported by the Bulgarian National Scientific Fund project КП-06-Н71/9 o f the Ministry of Education and Science, Bulgaria.

On a Spontaneous Polarization Induced by Chiral Additives in Smectic Liquid Crystals

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Keywords: liquid crystal, smectic, chiral additive, spontaneous polarization

In the present work the investigation of the value of induced spontaneous polarizatin P_s in liquid crystal (LC) systems of smectic matrixes with various chiral additives has been carried out. As investigated objects the following smectic C LC: $C_5H_{11}O-(OH)C_6H_3-CH=N-C_6H_4-C_5H_{11}$ {I}; $C_{10}H_{21}O-C_6H_4-CH=CH-C_6H_4-OC_{10}H_{21}$ {II}; and ferroelectric smectic C LC: $C_7H_{15}O-C_6H_4-C_6H_4-COO-CH_2C^*H(CH_3)C_2$ {III}; $C_8H_{17}O-C_6H_4-C_6H_4-C_2H_4C^*H(CH_3)C_2H_5$ {IV} were chosen. In our experiments, the LC test samples were filled in "sandwich" type cells, and glass surfaces were preliminarily given a planar orientation, the cell thickness was 20 μm. The precise measurements of temperature dependences of P_s in the range of phase transitions in the test samples were carried out by the Sawyer-Tower repolarization method [1,2].

Obtained experimental results of P_s for the LC systems under study have approximately 10 times greater value of P_s than the data P_s of ferroelectric LC {III} and {IV}, submitted in [3]. It is established the occurrence of the large value of spontaneous polarization in the LC system in which the composition`s molecular structure is not satisfied to obligatory conditions, imposed by theory on molecular structure for the occurrence of spontaneous polarization. In LC systems under investigation, the temperature range of the ferroelectric phase existence is also much wider. The essential role of short-range intermolecular forces during the ferroelectric phase transition is shown. A dimer model for increasing the value of spontaneous polarization is proposed.

Acknowledgements: This work was carried out within the framework of basic funding provided by the Higher Education and Science Committee of MESCS Republic of Armenia.

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Preparation and investigation of hemorphin peptide lyotropic liquid crystals in the presence of metal ions.

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Keywords: hemorphin peptide; liquid crystal phase;

Peptide molecules of various types can interact with various metal ions, controlling the structures and functions of many biological processes in organisms. Numerous studies in metallopeptide chemistry have been conducted with the main goal of developing synthetic peptide analogs that coordinate with metal ions through their functional groups to introduce special reactivity or construct nanostructures. On the other hand, different types of peptide molecules can undergo a process of self-assembly through non-covalent interactions between molecules and form a variety of liquid crystalline (LCs) structures with potential application in medicine [1]. The process of producing peptide molecules in mesogenic form, with lyotropic and thermotropic liquid crystalline phases, can be influenced by a variety of factors such as temperature, medium pH, metal ion concentration, and so on [1]. The current study aims to provide information on the behavior of hemorphin peptide derivatives in LC phases formed by molecules with different amino acid sequences and peptide bone lengths, as well as an understanding of how the self-assembly process can be controlled by interactions between molecules and other parameters such as the relative volumes of different parts of the molecules. The peptide LC phases were characterized under various conditions using IR and fluorescence spectroscopy, ζ-potential determination, peptide loading efficiency by liquid chromatography, and voltammetry. The studies described here would help to develop novel peptide LC molecules and control these LC structures by inserting metal ions with promising applications.

Acknowledgements: This study is funded by the European Union-NextGeneration EU, through the National Recovery and Resilience Plan of the Republic of Bulgaria, project № BG-RRP-2.004-0002, "BiOrgaMCT".

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Chemically Functionalized Spinorphin Peptide Nanosystems Mixed with Lyotropic Liquid Crystal Structures for Potential Application in Medicine

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Keywords: spinorphin peptides, nano-peptide, lyotropic liquid crystal (LC) structures

The development of anticonvulsant drugs poses a significant challenge to the global health sector. Spinorphin peptide derivatives are a class of new compounds that have recently demonstrated significant biological action in decreasing convulsions in in vivo tests. However, spinorphin peptide derivatives (SPDs) suffer from relatively low stability due to proteolytic and chemical degradation. As a result, carrier systems such as nano-peptides protecting these compounds are highly needed to achieve efficient biological action. On the other hand, the possibility of easing the process of passing through the blood-brain barriers of the mentioned compounds necessitates the search for suitable structures as carriers. In this work, we describe research on the potential of lyotropic liquid crystal (LC) structures as carriers for three spinorphin peptide derivatives and associated nano-peptide modifications. Cubic glycerol monooleate/water and hexagonal glycerol monooleate/oleic acid/water LC structures were tested. Both bulk gels were used, and discrete dispersed structures were investigated, i.e., cubosomes and hexosomes. Characterization of the initial LC structures without and in the presence of peptide and nano-peptide was performed by IR spectroscopy, x-ray scattering (SAXS), dynamic light scattering, ζ-potential, and peptide loading efficiency by liquid chromatography and voltammetry. The biological activity of peptide-loaded LCs was investigated in vivo using minimal inhibitory concentrations (MIC). The results show that the most hydrophobic peptide tends to induce an increase in negative curvature of the bulk cubic LC gel, thereby pushing the system towards a hexagonal structure.

Acknowledgements: This work was financially supported by the Bulgarian National Scientific Fund project КП-06-ДО-02/3 (title: New opioid peptide-nanoparticle conjugates: synthesis, characterization and neuropharmacological applications) of the Ministry of Education and Science, Bulgaria.

Study of the Influence of Molecular Structure Features on Mesophase's Thermal Stability and Formation in Nematic Liquid Crystals Using Dielectric Measurements.

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Keywords: liquid crystal, nematic, dielectric permittivity, thermal stability, phase transition

The results of the investigation of the dielectric response of the liquid crystal (LC) system to an external alternating electric field are presented. .The research object was chosen to be nematic LC: $\frac{C_7H_{15}-C_6H_4-COO-C_6H_4-CN}{Cr\xrightarrow{43^\circ C}NLC\xrightarrow{58^\circ C}IL}\{I\}$;$\frac{C_5H_{11}-C_6H_4-C_6H_4-CN}{Cr\xrightarrow{24^\circ C}NLC\xrightarrow{36^\circ C}IL}\{II\}$; $\frac{C_4H_9-C_6H_4-COO-C_6H_4-OC_6H_{13}}{Cr\xrightarrow{32^\circ C}NLC\xrightarrow{49^\circ C}IL}\{III\}$, as well as its systems with different concentrations of $\{I\}$and $\{II\}$. The measurements were conducted on oriented LC (with a thickness of the LC layer ranging from 10 to 20 μm) at low frequencies, where the orientation polarization changes in sync with the external field. A measuring field with an intensity of $E \approx 20\ V \cdot cm^{-1}$ was used, which is an order of magnitude smaller than the critical field.

A dependency of the thermal stability of the nematic phase on the system's composition has been obtained. Noticeably, the melting point of the investigated LC systems does not depend on the system's composition. However, unlike the melting point, the clearing point of the systems changes with variations in the concentration of components.

It has been found that the transverse component values of the dielectric permittivity in the nematic phase of NLC systems adhere to the law of additivity, whereas the behavior of the clearing point does not align with the mentioned law.

The temperature dependence on the magnitude $B(T) = (\varepsilon_\perp - n_\perp^2)(2\varepsilon_\perp + n_\perp^2)/3\varepsilon_\perp$, characterizing an average transverse dipole moment of molecules has been obtained using the Kirkwood formula [1] for the case of liquids consisting of rigid dipoles (where T-is the temperature; $n_\perp$- is the refractive index of the extraordinary ray in a LC medium).

It is shown that the value of B, slowly changing with temperature, increases abruptly near the $NLC \rightarrow IL$ phase transition, reaching saturation at the transition point. It's demonstrated that the jumps in $\varepsilon_\perp$ during the $NLC \rightarrow IL$ phase transition are attributed to the increasing alignment of transverse dipoles of neighboring molecules towards a parallel arrangement, confirming the Chandrasekhar correction [2] made in the theory for the static dielectric constants of NLC.The numerical approximation of the dielectric spectra of the investigated LC phases is performed.

Acknowledgements: This work was carried out within the framework of basic funding provided by the Higher Education and Science Committee of MESCS Republic of Armenia.

References:

[1] H. Frohlich, *Theory of Dielectrics,* (Oxford University Press, 1987), pp. 200.
[2] L. Blinov, *Sructure and Properties of Liquid Crystals,* (Springer Dordrecht Heidelberg London New York, 2011), pp.438.