International School of Liquid Crystals
18th Course

"Liquid crystal nanostructures and self-assembling: from organic electronics to metamaterials"

S I C L
SOCIETÀ ITALIANA CRISTALLI LIQUIDI

2nd School of the Italian Liquid Crystal Society

E. Majorana Centre for Scientific Culture, Erice (Italy)
Erice, 3 -10 July 2011

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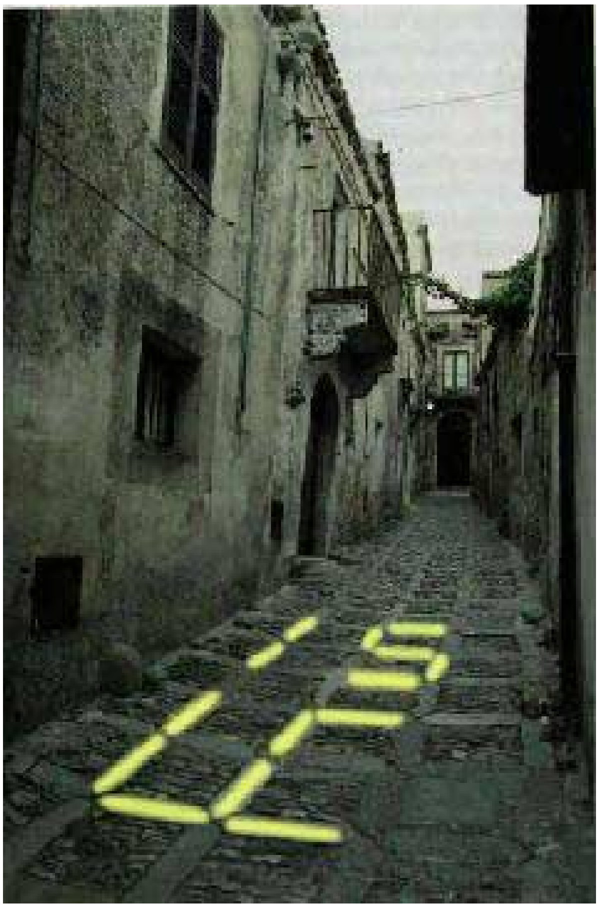

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Lecture 02	Philippe Barois	SELF-ASSEMBLY ROUTES TO METAMATERIALS FOR VISIBLE LIGHT
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Lecture 05	Bertrand Donnio	NANOSTRUCTURED LC ASSEMBLIES OF FUNCTIONAL CLUSTERS AND NANOPARTICLES
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Lecture 09	Dean R. Evans	STRESSED FERROELECTRIC NANOPARTICLES AND THEIR USE IN DISPARATE LIQUID CRYSTAL SYSTEMS
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X-ray methods for liquid crystals investigations

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Abstract of the lecture:

An X-ray scattering experiment is a common stopover on the way of a freshly synthesized liquid crystal towards fundamental or applied research. Indeed, the accurate knowledge of the microscopic structure of a LC material is always a precious piece of information that impacts all physical properties. The classical rules of crystallography of course apply to liquid crystals, but the specific properties of these fluid materials have interesting consequences on the experimental approaches and on data analysis. Large molecular repeat units generally imply small angle scattering (SAXS). In addition, fluidity, soft elasticity, local disorder or chirality, to name a few typical LC features, are responsible for diffuse scattering, broadening of Bragg peaks, gradients of local order or extinction of forbidden reflections that can be characterized by appropriate x-ray diffraction tools.

We review in this lecture a few experimental methods that are used in the determination of liquid crystal structures by x-ray scattering, such as:

- high resolution studies for lineshape analysis [1,2]
- x-ray reflectivity at LC interfaces
- grazing incidence diffraction in thin film geometries
- resonant scattering for contrast variation and the characterization of chiral structures
- X-ray photon correlation spectroscopy

Main references:

- **[1] Als Nielsen et al,** *Phys. Rev.* **B22**, 312 (1980)
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Self-Assembly Routes to Metamaterials for Visible Light

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Abstract of the lecture:

Metamaterials are artificial composites exhibiting extraordinary optical properties unknown in natural materials. These properties result from the enhanced electromagnetic response of engineered resonators much smaller than the wavelength λ of light travelling through them (meta-atoms). The basic challenge of the field lies in our capacity to design and fabricate such resonators. This challenge was beautifully taken up at Gigahertz and up to Terahertz frequencies by the design of split ring resonators (SRR) by Sir John Pendry in 1999 and the subsequent demonstration of extraordinary optical properties such as negative refraction or cloaking.

For visible light however, the SRR design and the related lithography techniques appear inappropriate. First of all, the effective medium condition (sizes $<< \lambda$) requires typical sizes of the resonators not larger than a few tens of nanometres. The fabrication of a metamaterial sample hence requires the assembly of more than 10^{12} nanoresonators per cubic mm! Self-assembly naturally appears as a first choice method to organize such a huge number of particles. On the other hand, the frequencies of visible light approach the plasma frequencies of metals so that metallic nanoparticles may constitute efficient nanoresonators. Indeed, the most recent advances in nanochemistry enable the fabrication of a large variety of finely engineered plasmonic nanoparticles of controlled size, shape, surface function, etc…

Associating the skills of nanochemistry (for the fabrication of plasmonic nanoresonators) and of soft condensed matter (for self-assembly of these nanoobjects) hence appears as a very promising route for the fabrication of nanostructured metamaterials operating in visible light.

We review in this lecture a series of metamaterial designs and of fabrication routes based on this approach.

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- **V. M. Shalaev,** *Nat. Photonics*, **1**, 41 (2007)

Physical properties and characterization of biaxial liquid crystals

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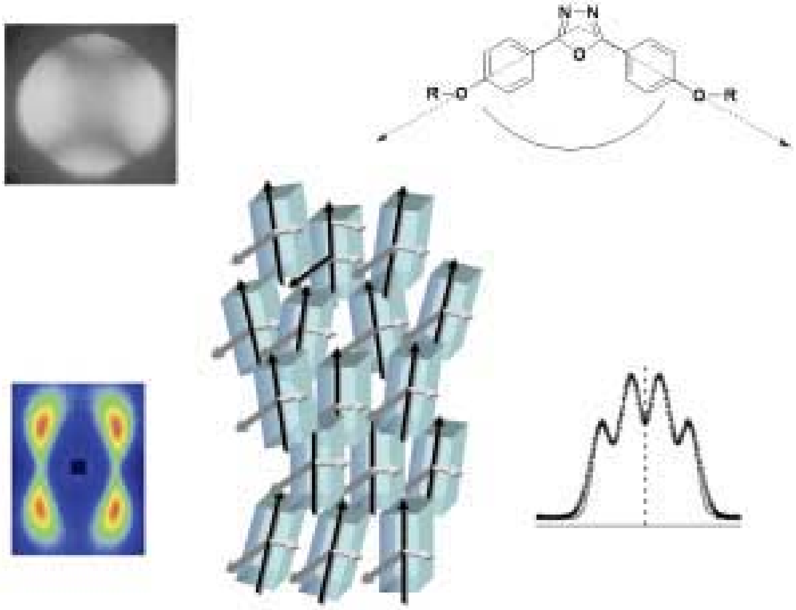
Biaxial liquid crystalline (LC) phases are of great interest for both pure scientific reasons and possible new technological applications. Several molecular systems of increased complexity have been synthesized so far with the aim of providing an incontrovertible evidence of phase biaxiality. Among them, it's worth noticing the biaxial nematic phases formed by bent-core LCs [1,2], tetrapodes [3] and LC polymers [4], as well as the biaxial smectic A phase observed in several thermotropic LCs [4,5]. Before going into details about the experimental methods used to discriminate between uniaxial and biaxial phases, several symmetry and orientational ordering concepts [6,7] will be reviewed (i.e. phase *vs* molecular biaxiality, …).

Experimental techniques typically used to investigate LCs, such as polarizing optical microscopy (POM), conoscopy [8], electro-optic measurements [9], X-ray diffraction [10] and calorimetry [2], are, in principle, sensitive to phase biaxiality. However, small values of the phase biaxiality and the influence of external fields in macroscopically aligning LCs often introduce complications and experimental limits. The analysis of data recorded by the above (sometimes complementary) techniques in terms of phase biaxiality is most likely performed in addition to detailed structural investigations [10] and spectroscopic studies, such as infrared [11], Raman [12] and NMR ones [1,6,7,13].



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Dendritic supermolecules: Synthesis, properties, & functions

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The hyperbranched motif is the most prolific, influential and fascinating pattern observed on earth, existing at all dimension length scales (from nm to km), and omnipresent in both the inert and the living worlds (crystals, metals, snowflakes, rivers, fractures, bacteria, virus, plants, trees, flowers, roots, corals, neuronic cells, nervous system, bronchial and blood streams, ….).[1] Intrigued by these highly symmetrical and compelling patterns reminiscent of fractals, mathematicians designed and developed complex recursive algorithms[2] with the aim to analyzing growth patterns and ultimately understanding specific functions found in the vegetal world. Equally inspired, chemists concomitantly started to imagine sophisticated iterative synthetic methods for the construction of structurally related artificial tree-like/cascade macromolecules. The elaboration of these aesthetically-challenging exotic architectures was at first essentially driven by simple synthetic curiosities and speculations, but quickly was motivated by the need to mimic and replicate these natural arborescent networks and to convey and exploit original functions and performances at the molecular level.[3]

Dendritic-like macromolecules now emerge as a key stage in the ongoing advances in the fields of supramolecular and macromolecular chemistry and self-assembly. Several competitive, conceptually very different, iterative synthetic methodologies (based on sequential synthetic elementary steps, repeated at each new generation eg convergent or divergent sequential modes, orthogonal and exponentional growths, etc…) have been developed for the preparation of these materials, leading to a myriad of dendroid-like structures, with increasing size and structural complexity. The ultimate architecture can be finely tuned by the "intrinsic dendritic connectivity" (core valency, branching degree, junctions and generations numbers).[3,4] Among these ramified architectures, dendrimers and dendrons have emerged as particularly versatile due to their high structural regularity (quasi-monodisperse), unique physical traits (combining those of both discrete low-molecular-weight materials and polymers), and controlled but geometrically-constrained three-dimensional branched topology. The diversity of the dendritic backbones combined to the high density, functions, and hierarchisation of inserted molecular moieties represent an attractive way of adding multiple functionality (e.g. high control of functions specificity, diversity, compartmentalization and hierarchy) and to elaborate materials with tuneable properties and/or with multi-properties (induced by cooperative and synergistic effects).[5-6] This chemical scaffold thus appears as nearly inevitable in the design of original self-assembling nano-elements,[7] catalysts,[8] functional materials[9] and bio-materials (bio-mimicry, drug, antimicrobial and gene delivery, encapsulation, imaging, diagnostics, therapeutics).[10] Molecular engineering of liquid crystals is also an important issue for controlling the self-assembling ability and the self-organizing processes of single moieties into periodically ordered nanostructures and still remains a fundamental challenge in material science.[11] Furthermore, ordered supramolecular assemblies can considerably enhance the functions of single molecules.[12,13] Research in the area of functional liquid-crystalline dendrimers consequently experiences outstanding developments, particularly due to the versatility of these original scaffoldings, in the elaboration of new LC multipurpose materials. These various aspects, eg synthesis, properties and functions will be discussed thoroughly.

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Nanostructured LC Assemblies of Functional Clusters and Nanoparticles

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Nanostructured Materials are a new class of materials which present some of the greatest potential for improving the performance and extending the capabilities of products in a number of industrial sectors. Research in this area aims at producing *nanoobjects* that are able to self-organize into periodic arrays and whose functions (optical, magnetic, electronic) can be addressed and manipulated by external stimuli. Synergistic collective modes and the emergence of new physical properties are also expected to benefit from the accurate control of the spatial assembly of these objects into ordered, periodic arrays. The principal advantage of this *bottom-up* approach is device miniaturization whereby the single object (or a small assembly) can perform the same task as a classical (macro) component. In this respect, optically/magnetically/electronically-active, nanometer-scale polymetallic clusters (PMC) and nanoparticles (NPs) arranged into low-dimensional 2D or 3D lattices constitute an attractive approach towards nanostructured materials for a wide range of potential applications including high density recording media, single-electron microelectronic devices and self-assembled metamaterials.

Our strategy for obtaining nanostructured arrays of small functional objects involves surface-hybridization of nanocrystals by structure-directing dendritic ligands, to give new functional hybrid materials. Since self-organization can only take place in systems that have some fluidity during the process, liquid crystals (LC) appear to be ideal candidates for promoting the arrangement of these small objects, whereas dendritic molecules provide structural versatility and functional hierarchy. The induction of LC mesophases of various magnetic core-shell hybrids, namely Mn12 SMM, Au@NP, QDs, and Fe_2O_3@NP, whose supramolecular arrangements and physical properties are controlled by their surface derivatization will be discussed.

Single-Molecule Magnets (SMMs) are much investigated for the development of high-density information storage systems or the implementation of quantum algorithms for computation. For both applications the control of the magnetic state is paramount. After a brief reminder of the fundamental properties of SMM, [1] our approach for controlling the magnetic anisotropy of Mn12 SMM ($[Mn_{12}O_{12}(L_i)_{16}(H_2O)_4]$) by surface hybridization and subsequent supramolecular organisations will be described. In particular, how pro-mesogenic ligands can provide a means for finely tuning the molecular geometry of the SMM without deleterious effects on the magnetic behaviour: they can be rendered mesomorphic by surfacial acetates substitution with designed gallic-based derivatives, hence providing self-organized SMM with various low-dimensional orderings [2]. Comparison of the bulk magnetic properties of the series provides evidence of a striking correlation between molecular structure and coercitive field. All of these results confirm that the deliberate distortion of the molecular structure can indeed influence the final magnetic properties. We will also show that the magnetization of a non-photo-sensitive SMM can be driven between different stable magnetic states by simply using the adequate combination of visible light irradiation and magnetic field conditions. The irradiation at optical wavelengths can trigger an increase or a decrease of the magnetic moment of a SMM, opening prospects as a means of controlling molecular magnets through stimulated superradiance.

Large alkanethiol-coated Au@NP can spontaneously self-organize in 2 or 3D, but NP with diameters smaller than 10 nm do not. Dendronized, 2nm gold particles show a fluid cubic mesophase (analogous to NP superlattices) and are ferromagnetic up to 400K [3]. It will be showed how the LC order interacts with the magnetic properties, as evidenced by the onset of an unusually slow relaxation of the remnant magnetization as the order develops. It is tentatively suggested that there might be a spin glass-like type of magnetism at the individual particle level and that the observed relaxation is under the influence of the mesophase *via* ligands orientation (LC mesophases). This approach has been extended to, mesogen-hybridized monodisperse QDs and iron oxide nanocrystals display optical/magnetic and mesomorphic behavior [4]. It will be showed how the magnetic properties are affected after surface-hybridization, suggesting modification of the magnetic anisotropy and/or the surface state of the hybrids has taken place.

Main references

[1] SMM: single molecule magnets are molecular compounds able to retain a stable magnetization at the molecular level, without any need for domains, walls, or exchange interaction between neighbouring magnetic entities. They are envisioned as candidates for the storage and processing of information at the molecular level.

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Traditional and novel NMR techniques for LC systems

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The particular strength of NMR is to report on the behaviour of the molecules in a liquid crystalline sample. This includes their translational and rotational motion as whole molecules, and the orientational order that this produces. The molecules which form liquid crystalline phases are almost always flexible by virtue of rotations about chemical bonds. NMR reveals the presence of this intramolecular motion and is able to quantify its effect on orientational order. An overview will be given of recent experimental developments which widen the range of liquid crystalline systems that can be studied by NMR.

NMR studies of solutes in liquid crystalline phases

A solute is usually defined as being a minor component in a mixture, and for liquid crystalline samples studying the behaviour of the solute may be driven by a wish to obtain information on the liquid crystalline phase, when it is described as a probe. Using a probe may be driven by a need to simplify the problem of interest, such as the nature of the phase, the alignment of the mesophase director by applied fields. Or the aim of the experiment may be centred on the solute, its structure, conformation, orientational order, and perhaps also its chirality. Examples of both kinds of study will be presented.

Stressed Ferroelectric Nanoparticles and Their Use in Disparate Liquid Crystal Systems

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Ferroelectricity refers to the property of certain materials possessing a spontaneous polarization, i.e. electric dipole, in which the dipole orientation can be controlled by an electric field. The influence of the electric field and heating can have different effects, which are application specific. In the form of nanoparticles, ferroelectric materials have proven to be useful in many liquid crystal (LC) devices, where the addition of low concentrations of nanoparticles fabricated from inorganic ferroelectric materials has a profound effect on the electrical [1-3] and optical properties of LC systems [4-6]. The electro-optic response and the field effects of the resulting composite medium is usually significantly different from that of the constituent ingredients, which has attracted the interest of several disparate (LC, photonic, and meta) scientific communities.

Until recently, it was believed that ferroelectric materials lose their spontaneous polarization at smaller particle sizes, e.g. less than 100 nm for $BaTiO_3$ [7,8]. In the lecture, it will be shown that $BaTiO_3$ particles of a size less than 10 nm do possess ferroelectricity; the physical reason will be explained. Topics related to these organic-inorganic hybrid LC systems will include: fabrication and harvesting of ferroelectric nanoparticles for inclusion into liquid crystal media [9,10], experimental and theoretical methods to verify and quantify ferroelectricity [10,11], experimental methods to characterize ferroelectric nanoparticles in both isotropic and anisotropic liquids [11], and the dynamics of isolated and aggregated nanoparticles and their effect on the spontaneous polarization [11]. The physical mechanism of the interaction between liquid crystals and inorganic ferroelectric nanoparticles will be shown. In addition the lecture will address different mechanisms by which inorganic substrates generate localized and bulk electric fields, and the interaction between surface fields and adjacent liquid crystal layers. The controversy over the reproducibility will be discussed and methods to overcome this irreproducibility will be explained.

From a device perspective, two disparate technologies will be discussed: 1) beam coupling, where the ferroelectric nanoparticles respond to a photo-generated electric torque [4], resulting in a more sensitive liquid crystal modulation and larger optical gain; and 2) display applications, where the nanoparticles create a DC bias, thus reducing voltage requirements (Freedericksz transition) [6].

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Introduction to liquid crystals as semiconductors and determination of their transport properties

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The performances of optoelectronic and photonic devices based on organic materials, when compared to their more traditional inorganic counterpart, still lag behind. This is a consequence of the poorer level of several functional features such as, for example, charge mobility or photogeneration efficiency. Nonetheless, the development of molecular or polymeric semiconductors is currently a hot topic and this can be understood in terms of a series of considerations:

- With Carbon-based chemistry it is possible to design and synthesize structures with tailored properties
- Non-covalent intermolecular forces can be used to obtain complex functionalities
- Thin films with controlled nano-morphology can be obtained via different techniques, including ink-jet printing
- Low temperature processing compatible with flexible, lightweight substrates is available
- Materials and processes are potentially low cost, even for large area manufacturing

The first subject touched during the lecture will be the main models used to describe charge transport in organic materials. In particular, the main ideas behind, and results of, the Marcus Electron Transfer theory and the Gaussian Disorder formalism will be introduced and discussed. The main advantages of liquid crystals as semiconductors will then be illustrated by discussing several recent literature results.

The description of the techniques used to measure charge mobility will be the subject of the second part of the lecture. Several commonly used techniques (Time-Of-Flight, Space-Charge-Limited-Current, Time-Resolved Microwave-Conductivity, Carrier Extraction by Linerly Increasing Voltage, Field-Effect-Transistor Characteristics, TeraHertz Spectroscopy) for measuring mobility will be described and contrasted, with the aim of clarifying not only their implementation but also their limits, their respective advantages and disadvantages and the comparability of their results.

The last section of the lecture will deal with charge photogeneration, photoconduction and photorefractivity in mesophases.

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Topological Defects (I + II)

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Abstract of the lecture.

First identified through the beautiful textures of their defects, liquid crystalline materials may very well be the ideal proving grounds for exploring notions of broken symmetries, associated Goldstone modes, phenomena akin to the Higgs mechanism, and, of course, topological defects. Indeed, the subjects of topological defects and liquid crystals are so intertwined that it is difficult to see how a thorough understanding of one could be garnered without knowledge of the other.

The homotopy theory of topological defects is a powerful tool for organizing and unifying many ideas across a broad range of physical systems. Recently, experimental progress has been made in controlling and measuring colloidal inclusions in liquid crystalline phases. The topological structure of these systems is quite rich but, at the same time, subtle. Motivated by experiment and the power of topological reasoning, we review and expound upon the classification of defects in uniaxial nematic liquid crystals. Particular attention is paid to the ambiguities which arise in these systems, which have no counterpart in the much-storied XY model or the Heisenberg ferromagnet.

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How the Cholesteric Got its Stripes

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Abstract of the lecture.

We present a microscopic analysis of the instability of the nematic phase to chirality when molecular chirality is introduced perturbatively. We show that for central-force interactions the previously neglected short–range biaxial correlations play a crucial role in determining the cholesteric pitch. We propose a pseudoscalar strength which quantifies the chirality of a molecule. The fundamental issues of symmetry related to chirality are discussed and applied to simple situations relevant to liquid crystals. We show that any chiral measure of a geometric object is a pseudoscalar (invariant under proper rotations but changing sign under improper rotations) and must involve three-point correlations that only come into play when the molecule has at least four atoms. In general, a molecule is characterized by an infinite set of chiral parameters. The authors illustrate the fact that these parameters can have differing signs and can vanish at different points as a molecule is continuously deformed into its mirror image. From this we conclude that handedness is not an absolute concept but depends on the property being observed. Within a simplified model of classical interactions, we identify the chiral parameter of the constituent molecules that determines the macroscopic pitch of cholesterics.

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Liquid-crystals-plasmonic metamaterials for advanced optical processing

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Abstract

Liquid crystals and plasmonic materials possess unique optical properties and have been actively investigated in various contexts. In particular, micro- and nano-structures such as photonic crystals and metamaterials that possess novel tunable and/or nonlinear optical properties have been theoretically and experimentally demonstrated [1-6]. Most reported experimental studies employ ac electric field induced director axis reorientation or temperature-controlled birefringence modification [2,3]. These electro-optical tuning mechanisms are characterized by switching times ranging on the order of milliseconds under typical applied field strength as in conventional display device.

On the other hand, nonlinear all-optical or self-action mechanisms, in which the desired changes in optical refractive indices or birefringence are generated by the light intensity itself, are in many situations more preferable since they do not require any electrode, and the incident light can impinge at almost any desired angle. In this lecture, we present a critical review of the nonlinear optical responses of nematic liquid crystals (NLC) associated with short pulsed laser induced order parameter and birefringence modifications, and describe how the plasmonic particulates/nanostructures embedded in them could enhance the nonlinearities and provide an ultrafast switching mechanism. Experimental studies conducted with absorbing as well as transparent nematic liquid crystals have demonstrated the feasibility of sub-microseconds – nanoseconds all-optical one-way switching of nanoseconds pulsed laser at various wavelengths spanning the entire visible – near infrared regime (400 nm - 1550 nm) [4]. These effects may be useful for developing tunable metamaterials and other materials/structures impregnated with nematic liquid crystals; they could also be applied to realize faster-response version of many coherent optical image processing applications demonstrated previously with slower mechanisms [1].

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Nematic biaxiality in thermotropic liquid crystals

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The question of nematic biaxiality has exercised the LC field since this phase was first proposed more than 40 years ago. For a lyotropic system phase nematic biaxiality was first observed in 1980 and these initial results have been confirmed and extended to further materials for a number of lyotropic systems.

For thermotropic nematics the picture is certainly more varied. A number of theoretical and synthetic approaches have been pursued to predict and obtain experimentally biaxial nematic systems. These activities have been and still are intimately connected to the development and refinement of methods for the unambiguous identification of nematic biaxiality.

In this presentation the developments over the past few years will be reviewed from a synthetic perspective and the current approaches to obtain thermotropic biaxial nematics will be outlined.

In particular, the advantages and drawbacks of approaches based on side-chain polymers, dimers, tetramers and bent-core molecules and that based on mixtures of rid-and disc shaped mixtures will be discussed and recent results will be presented.

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The chemistry of self-organized nanocomposites for the design of metamaterials

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Classically metamaterials are associated with concepts focused in the main on designs with properties in the radio-wave spectrum. Only in recent years efforts have concentrated too on concepts with metameterials properties in the visible range of the electromagnetic spectrum. In this presentation the work based on the design and investigation of materials with metamaterials properties based on the self-assembly of hybrid nanocomposites is presented. Crucial features are the the design and synthesis of nano-composites consisting of gold nanoparticles and liquid crystal orgnaic groups which assemble in a cntrolled manner
The investigation of small LC functionalized nanoparticles leading to systems where the self assembly behaviour is determined by an interplay of the particles' structure and the self-assembly behaviour of mesogens will be reported and some structure properties correlations with dendrimers will be made. The correlation between the self-assembly behaviour of the nanoparticles with 2D and 3D assembly and their size and the degree of mesogen coverage will be discussed. The impact of the size of the nanoparticles and the self assembly behaviour on the optical properties, using preparations of thin films will be reported and discussed.

Liquid crystal semiconductors and applications I and II

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Since the first demonstration of Organic Light-Emitting Diodes (OLEDs) based on conjugated small organics and main-chain polymers, interest in the field of organic electronics has expanded enormously with applications in solar cells, plastic electronics as well as displays. Charge-carrier transport and light-emission in or organic semiconductors depend not only on the orbital energies and wave-functions of the individual molecules or polymer chains, but also on intermolecular interactions, determined by the thin film morphology. Self organisation by the formation of liquid crystalline phases is considered a key strategy to control the order and packing of organic semiconductors and so improve their charge transport and optical properties.[1-4] Another advantage of liquid crystallinity is the ability to form monodomain samples with uniform alignment and without defects caused by grain barriers.

We introduce the basic principles and device configurations of organic field-effect transistors (OFETs), OLEDs and photovoltaics and identify the key parameters used to measure performance. The applications areas of these devices are outlined. We discuss the use of polymer liquid crystals, reactive mesogens and columnar liquid crystals in OFETs, focussing on materials, self-organisation and device features. Optoelectronic devices such as organic photovoltaics and OLEDs require optimisation of both charge transport and optical properties and we identify the various trade-offs involved. Luminescent liquid crystals are then reviewed for polarised electroluminescence and pixellated OLEDs. We update progress on the surface alignment of liquid crystalline semiconductors as a strategy to obtain monodomain devices without defects or devices with spatially varying properties. We investigate two different approaches, based on columnar and reactive liquid crystals respectively, to develop organic photovoltaics. The processing of liquid crystals in semiconductor devices is then discussed. Finally the significance of all of these developments is assessed.

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Optical Metamaterials: From Basic Physics to Applications

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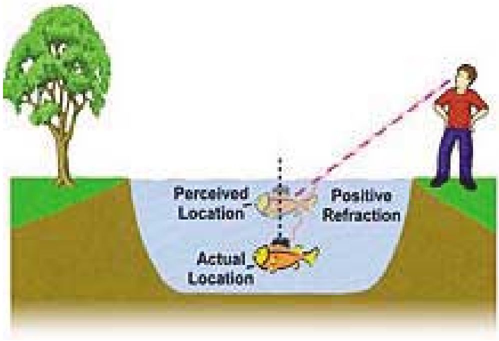
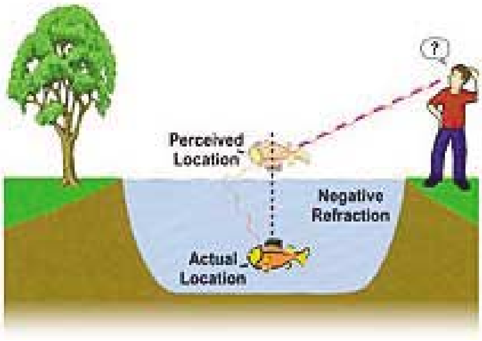
Metamaterials form a new class of artificial, composite materials whose response to waves (either electromagnetic, or acoustic) is extraordinary and unknown to natural materials. Since the first realisation of a metamaterial, in 2000, this very recent field has been booming and has brought some of the most spectacular physics experiments of the past decade.

Metamaterials are promising for a diversity of optical/microwave applications, such as new types of beam steerers, modulators, band-pass filters, superlenses, microwave couplers, and antenna radomes. In order for its structure to affect electromagnetic waves, a metamaterial must have structural features at least as small as the wavelength of the electromagnetic radiation it interacts with. In order for the metamaterial to behave as a homogeneous material accurately described by an effective refractive index, the feature sizes must be much smaller than the wavelength. For visible light, this is on the order of one micrometre; for microwave radiation, this is on the order of one decimetre.

In these lectures, we will endeavour to present an overview of the field, first by recounting the fairytale-like story of its beginnings, then by presenting the most striking realisations and potential applications from metamaterials, and finally by pondering over the huge challenges that are still ahead.





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Differential Geometry and Topology of Nematic Defects

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The lecture is intented to illustrate the interplay bewteen the differntial properties of an orientable surface and the defects of a nematic liquid crystal deposited upon it. The nematic order, and its lack that characterizes defects, will be described in a tensorial formalism appropriate to this setting. I will recall old concepts such as geodesic curvature, Gauss-Bonnet formula, Levi-Civita's parallel transport, Euler characteristics and genus of a surface. I will show how these may justify a new, purely tensorial representation of the topological charge, which on a flat syrface would just be the classical winding number. If time permits, I will also show how these concepts have a bearing on an elastic theory for nematic shells, a topic which has recently become very fashionable in liquid crystal science.

Nematic shells are thin films of nematic liquid crystals deposited on colloidal particles whose boundary enforces a tangential degenerate anchoring on the nematic molecules deposited upon it. Depending on the genus of the colloid's boundary, defects in the local nematic order may be unavoidable. If, as it has already been proposed, defects on nematic shells may play the role of ligands' anchors, new supramolecular organizations could be imagined whose building blocks are colloidal particles instead of molecules. In this new chemistry, the number of stable defects would be the equivalent of the valence of classical chemistry. There is a purely geometric way to control the colloidal valence as well as there are geometric mechanisms able either to aggregate or to separate defects.

Describing Molecular Organizations in Liquid Crystals.
Order Parameters, Distributions and All That

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Soft matter comprises a variety of condensed matter systems like liquid crystals, polymers, colloids and several biosystems, whose importance largely derive by (i) properties intimately related to their molecular organization and (ii) the fact that their structure can be easily modified thermally or by the intervention of external fields. Understanding these systems requires describing their microscopic structure in terms of quantities like order parameters and distribution functions [1,2] that can, at least in principle, be determined by experiment and/or theory and computer simulations.

In this lecture we discuss some amongst the most important of these quantities and provide some examples of their experimental determination.

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Computer Simulations of Liquid Crystals. An Introduction

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The determination of observable properties starting from molecular models requires the use of computational methods rather demanding in computer resources. It is thus not surprising that these techniques have received a great impulse in the last few years, together with the development and availability of new and more powerful hardware and software platforms. In this talk we plan to describe the essentials of the two most important current simulation methodologies: Monte Carlo and Molecular Dynamics [1,2] and to show some examples of their application to various liquid crystal models ranging from lattice [3] to molecular (Gay-Berne) [4,5] and atomistic [6] models showing what they can now achieve both in descriptive and predictive terms.

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Introduction to nematic colloids

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Dispersion of particles in nematic phases with the intention to form colloidal superstructure is a relatively new field [1]. In this introduction we describe basics of nematic solvent and typical structures with dipolar and quadrupolar symmetry arising after dispersing spherical particles in the solvent with orientational order [2]. Size and anchoring effects on the stability of the defects and their effective interaction are described and related to the formation of regular 1D, 2D, and 3D structures [3]. Further the interaction based on the entanglement of particles by disclinations is introduced [4,5]. Formation and classification of simple nematic braids is briefly discussed [6].

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Chiral nematic colloidal superstructures

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In this lecture colloidal dispersions in simple cholesteric and cholesteric blue phases will be discussed. After a brief introduction of phases we first focus our attention to deformations induced by spherical particles in the cholesteric ordering. Particular attention will be paid to dispersions with particles larger than pitch. Interaction between inclusions and possible entangling is examined [1]. Further formation of knots and links leading to 2D braids in a twist cell is described [2]. In contrast to simple cholesteric structures the blue phases I and II that possess networks of disclinations are examined as possible trapping systems for small colloidal particles [3]. Crystalline arrangements of colloidal particles and limitations due to size and surface anchoring of inclusions will be discussed. Finally the effect on the blue phase stability diagram will be described.

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