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Keynote

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Electric conductivity in liquid crystalline calamitic, discotic and polymer monolayers at air-solid interface Kattera A. Suresh

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We present our studies on the electrical conductivity in liquid crystalline calamitic, discotic and polymer monolayers at air-solid interface. The monolayer films were formed at airwater interface and then deposited on conducting substrates by the Langmuir-Blodgett (L-B) technique. The films were studied by atomic force microscope (AFM) and the current-voltage (I-V) measurements were performed with a current sensing atomic force microscope (CSAFM). The I-V characteristics showed a non-linear behavior for all the systems. The monolayers of calamitic mesogens, 9 cyanobiphenyl (9CB) and 10 cyanobiphenyl (10CB) were deposited on highly oriented pyrolytic graphite (HOPG) substrates. The analysis of the I-V curve based on Simmons approach showed a direct to injection tunneling transition. The monolayer of discotic material pyridinium tethered with hexa-alkoxy triphenylene (PyTp) was deposited on gold coated mica substrate. The current measurement and its analysis showed that for the PyTp monolayer, the charge transport was through injection tunneling. The polymer material based on 2, 6-dihydroxy-3, 7, 10, 11-tetraalkoxy-triphenylene (PHAT) shows discotic columnar phase. The monolayer of PHAT was deposited on gold coated mica substrate. The analysis of the I-V curve showed the charge transport to be direct tunneling. We discuss the transport mechanisms in our systems compared to others reported in literature.

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Invited Talks

Thermodynamic models for the phase transition properties in liquid crystals

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We shall discuss the application of thermodynamic models, based of Landau-de-Gennes type free-energy density expansion, to explain the phase transition behavior of achiral and chiral (ferroelectric, antiferroelectric, bent-core) liquid crystals.

Liquid crystals in photovoltaics: A new generation of organic photovoltaics Sandeep Kumar

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Liquid crystals have recently gained significant importance in organic photovoltaics. Power conversion efficiency up to about 10% has reached in solar cells incorporating liquid crystals. In this talk, I would like to presents an overview of the developments in the field of organic photovoltaics with liquid crystals. The talk will also include our recent research work on the preparation of solar cells with discotic liquid crystals. An outlook into the future of this newly emerging, fascinating and exciting field of self-organizing supramolecular liquid crystal photovoltaic research will be provided.

C₃-Symmetric, (n, π-cojugated)-Discotics: C_{3h} –Tris (ketohydrozone)s - The Tautomeric Forms of Tris(azo-enol)s Rashmi Prabhu, Doddamane S. Shankar Rao, S. Krsihna Prasad and Channabasaveshwar V. Yelamagad

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A new class of (n, π -cojugated) disk-like liquid crystals namely, tris(keto-hydrozone)s motifs - the tautomers of tris(azo-enol)s, have been synthesized quantitatively *via* one-step triple azo-coupling reaction. Optical, calorimetric and X-ray diffraction studies evidence their self-assembly into fluid columnar structure wherein the tris(hydrozone) cores, stabilized by resonance-assisted intra-molecular H-bond forces, segregate into indefinitely long columns arranged in two-dimensional array of rectangular or hexagonal symmetries. Notably, the thin films of the fluid/frozen columnar structure show photoluminescence in NIR wavelength regime. Their electrochemical behavior has been well-demonstrated as well.

Non-aqueous lyotropic liquid crystalline phases as a water free soft template and drug carrier <u>Ravi K. Shukla^{1, 2} and K. K. Raina^{2, 3}</u>

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Aqueous lyotropic systems are well studied in the literature and exploited for the variety of applications in the key area of biology, cosmetics, pharmaceuticals and nanotechnology. However, the lack of stability with passage of time and at higher temperature hinders their use in the device applications. To improve this issue we developed some lyotropic phases by using nonaqueous solvents. Anionic, cationic and non-ionic surfactants [sodium dodecy] sulfate SDS (CH₃ (CH₂)₁₁OSO₃Na)] [cetylpyridinuium chloride CpCl ($C_{21}H_{38}ClN$) and cetyltrimethylammonium bromide CTAB ($C_{19}H_{42}NBr$) and Tween20] and non-aqueous solvents like ethylene glycol and formamide were considered to develop the lyotropic phases. Distinct crystalline and liquid crystalline phases were observed from these systems. In this talk we will highlight how the nature of surfactant, counter ions, chain lengths, cohesive energy, and dielectric constant influence development of these phases and their physical properties. The advantages of nonaqueous lyotropic phases over the aqueous lyotropic phases will also be discussed. Such water-free stable lyotropic phases are especially attractive to engineer usual and hygroscopic nanoscale materials for targeted applications. The second part of this talk will be devoted to explore the biological applications of these mesophases and highlight their scope as drug vehicles.

Key-words: Lyotropic liquid crystalline phases, anionic, cationic and nonionic surfactants; soft templates; drug delivery.

Solvent Induced Structures of Soft Matter Yashwant Singh

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With the help of few examples the role played by solvents in creating patterns of solutes which constitute soft matter will be elucidated. Can have we a theory for such emergent structures? Attempt will be made to answer this question.

Structure and function of lipid droplets; and why this might be interesting to the LC community Mona Mirheydari¹, Sewwandi S. Rathnayake², Elizabeth K. Mann¹, and <u>Edgar E. Kooijman²</u>

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Lipid droplets are intracellular particles consisting mainly of neutral lipids, triglycerides and cholesterol esters, coated with a phospholipid-protein monolayer. While much research has focused on an understanding of lipid droplet biology much less is currently known about the structure, and formation, of lipid droplets, and how proteins interact with the unique phospholipid monolayer-neutral lipid interface. Our work has focused on understanding why lipid droplet binding proteins bind to this interface. This is an important question as there are far more lipid membranes in cells than lipid droplets. In this talk I will discuss our current understanding of lipid droplet structure and formation, and what we are doing to contribute to this growing field [1]. Specifically, I will discuss our work with our homebuilt liquid droplet interface. Additionally I will discuss some ways in which the liquid crystal community might be able to contribute to this growing and important field in biology.

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Highly improved efficiency in bulk heterojunction photovoltaic cells made from carbazole copolymer and fullerene derivative with a layer of columnar discotic liquid crystalline material Manisha Bajpai¹, Neelam Yadav¹, Ritu Srivastava², Sandeep Kumar³ and <u>Ravindra Dhar¹</u>

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In our effort to prepare organic flexible solar cells using discotic liquid crystals (DLCs), bulk heterojunction photovoltaic cells based on composites of copolymer Poly [N-90-heptadecanyl-2,7-carbazole-alt-5,5-(40,70-di-2-thienyl-20,10,30-benzothiadiazole)] and the fullerene derivative, [6,6]-phenyl C71-butyric acid methyl ester with an inserted laver of columnar DLC between the interface of active and hole transporting layers have been fabricated. Different hole transporting layers deposited on indium tin oxide substrates such as poly (3,4ethylenedioxythiophene)-poly (styrenesulfonate) or molybdenum trioxide has been used in these devices. All the cells with inserted DLC layer have shown far better performance than the reference cells. Power conversion efficiency of 5.2% has been obtained for the photovoltaic solar cells having self-organized DLC layer of 30 nm thickness under one sun condition which is substantial jump as compared to earlier reports. The mobility of holes in the HAT4 inserted devices was found to be of the order of 10^{-6} cm²/V-s due to which high values of current density was achieved. The effect of variation of the thickness of DLC layer and annealing on the photovoltaic parameters of these devices has also been studied. Our effort is to further enhance the efficiency by doping nano materials in the columns DLCs.

Keywords: bulk hetro junction, solar cell, liquid crystals, mobility, efficiency.

Ester-Type Banana shaped liquid crystalline compounds containing Bis Naphthyl Moieties: synthesis and characterization

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It has been shown that not only rod-shaped (calamitic) or discotic molecules form liquid crystals, but bent core (Bowlike or Banana- shaped) molecules do also [1]. This discovery has opened up a major new and exciting dimension in the Science of thermotropic liquid crystals. Similar findings, with broad implications for the general field of soft condensed matter, include the observations of ferroelectricity and spontaneous chiral symmetry breaking in smectic phases composed of molecules that are not intrinsically chiral [2,3].

In the present study, we report the synthesis and characterization of two series of symmetrical banana shaped compounds with 1,3-disubstituted benzene (Resorcinol) as the central unit. These materials combine by ester (-COO-) linkages with different terminal alkoxy chain and changes the position of fused (bis naphthyl) ring. The position of the (bis naphthyl) ring does effect the thermotropic properties of bent core molecules.

The synthesized bent core compounds of both series have been characterized by usual spectroscopic techniques. The mesomorphic behavior was investigated by polarizing optical microscopy (POM) and differential scaning calorimetry (DSC). All the compounds of both series exhibit nematic phase and monotropic/enantiotropic in nature.

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Critical behavior of birefringence in the vicinity of the smectic-A –smectic-C phase transition: Crossover from 3D-XY critical to tricritical behavior

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Classical liquid crystal phases are characterized by broken symmetries and may be utilized to explore the complex and beautiful relationship in nature between symmetry and spatial dimensionality at phase transitions. The smectic-A (Sm-A) and smectic-C (Sm-C) phases can be described as orientationally ordered fluids with quasi-long-range one-dimensional mass density waves either parallel (Sm-A) or inclined (Sm-C) to the unique orientational axis. The transition between the Sm-A and Sm-C phases involves the breaking of a continuous rotational symmetry. During the last four decades, many high-resolution heat capacity, volumetric and X-ray studies have been devoted to the smectic-A-smectic-C (Sm-A-Sm-C) phase transitions in a wide variety of mesogens and the centre of attention is the critical exponents for determining the universality class of this transition. But high resolution birefringence (Δn) data showing critical anomaly in the vicinity of Sm-A-Sm-C transition is still scanty. In most of the cases the resolution of the data available in literature in the vicinity of the transitions from birefringence measurements are quite insufficient for a faithful manifestation of the critical behavior near the phase transition region.

In this work, high-resolution birefringence (Δn) measurements have been carried out to probe the critical behavior at the smectic-*A* –smectic-*C* phase transitions in a binary system consisting of the second and seventh homologs of the 5-alkyloxy-2-(4-nonyloxy-phenyl) pyrimidine series. The critical behavior of this transition has been explored with the aid of a differential quotient extracted from the Δn values [1]. Our analysis resolves a long-standing puzzle about the critical behavior of this phase transition. The results obtained reveal that both the *N*–Sm-*A* and Sm-*A*–Sm-*C* transitions can be driven from second order towards a first-order nature and follow two distinctly different curves, with decreasing *N* and Sm-*A* ranges respectively. This work quantitatively shows that the origin of such critical behaviour is a unique feature in the respective phase transitions. Its applicability ranges from phase transitions in soft condensed matter physics to thermal phase transitions of in subatomic physics.

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Room Temperature Discotic Nematic Liquid Crystals: Design strategy

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The disc shaped molecules showing nematic phases (i.e. N_D phase) are rare but of utmost importance in many display device applications. They have received particular interest since their commercialization as optical compensation films to enhance the viewing angle of commonly used liquid crystal (LC) display based on polymerized nematic discogens. Unfortunately, among the limited number of discotic nematogens, most are accompanied by high temperature N_D phases and in a narrow range of mesophase temperature. However, for all practical purposes N_D LCs at room temperature are highly desired. In this talk, I will present a new strategy for the design of a room temperature N_D LC dimer derived from two incompatible disc-like mesogenic cores linked *via* flexible alkyl spacers. Unlike various approaches reported so far in the literature forming N_D phases, we found that the flexibility of the spacer between the two cores leads to folding of the dimer into a composite disc giving rise to the formation of a room temperature N phase. Several other combinations with similar discotic units forming tetramer and trimers will also be presented as a comparison.

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Electric field driven reorientation, propelling and spinning of anisotropic microparticles in nematic liquid crystals Surajit Dhara

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In this talk I will present and discuss some of our recent experimental results on the electric field driven reorientation, propelling and spinning of birefringent micro sheets in nematic liquid crystals. For a fixed direction of applied field in the isotropic phase, there are two critical fields above which the micro sheets show two orientations. In the nematic phase, it shows three rotations in both planar and homeotropic cells. These orientations are observed at varying voltage and wide time scales and explained based on the competing effect of the electric, elastic and viscous torques. In case of electric field driven propelling and spinning we found that the linear velocity and the angular frequency is proportional to the square of the applied electric field and they strongly depend on the frequency of the applied field. The results are explained based on the theory of liquid crystal enabled electrophoresis.

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Dendrimers as Cores and as Peripheries in Modifying Macromolecular Functions

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Dendrimers are hyper branched macromolecules, in which the branching occur through-out the structure. A monodispersed macromolecular structure results when there is no truncation in the branching pattern, which runs through branches-upon-branches. Monodispersity is an appealing structural feature of dendrimers that helps to correlate structure-function properties, when the dendrimer is incorporated with functional moieties either at the core or at the branches or at the peripheries. In efforts to delineate the role of dendrimer structures on functional properties, two approaches were undertaken in a programme. In the first approach, a poly(ether imine) (PETIM) dendrimer series was functionalized with mesogenic cholesteryl moieties at their peripheries. The functionalization included dendrimer generations one to three and a variation in the alkyl linker constituting the dendrimer structure. A detailed study of the mesophase properties of the series reveal that the alkyl linker constituting the dendrimer leads to profound changes in the mesophase structures, even when the number of cholesteryl moieties at the peripheries remains uniform. Continuing studies also show that in addition to the linker type, the functional moiety which connects the mesogen with dendrimer core exerts influence on the mesophase structures. Changes in liquid crystal (LC) properties suggests that a particular generation of a dendrimer alone modifies the functions in ways hither-to unknown, as opposed to such functional modifications known so far only for dendrimers of varying generations.

In the second approach, dendrons of first and second generations in the poly(alkyl aryl ether) series form side chains of poly-ene-yne polymer backbone. Presence of dendrons elevates the functional properties of the polymer; one of them is the thermochromism property. Such a property is significantly enhanced when the polymer backbone is grafted with dendron blocks. Features of dendrimer modified LCs and chromogenic polymers will be presented.

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Liquid crystal-nanoparticle hybrids: realization of restricted geometries and enhanced properties

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Nanoparticles have attracted great interest because of their unique physical and chemical properties based on the quantum-size effects, with potential to serve as novel materials for electronics, photonics, and magnetic devices. For optimal usage, it is desirable to control and tune the spatial arrangement and distribution of the nanoparticles. On the other hand, liquid crystals (LCs) as self-organized organic materials exhibiting long-range order, cooperative effects, and anisotropic nature in optical and electrical properties, while having fluid like order in one or more dimensions are naturally the media to achieve such an arrangement of the nanoparticles (NPs). Thus, the LC-NP hybrids, being the combination between the mature field of LC, with its structural diversity on a molecular/supramolecular level, notwithstanding the demonstrated impact on the display technology, and the fascinating nanoparticles with myriad behaviour, are very promising to study inorganic-organic particle interaction as well as interesting applications.

On another front, LCs confined to nanodimensions has entered a new and exciting era of complex geometries that are more random in nature. The intricate mechanisms which govern the physical properties of LC confined to well defined geometries, as well as to more complex and random ones, have revealed various properties and effects not observed in the same substances when they are in the bulk. Of specific interest are confinement achieved by (i) dispersing silica particles of a few nm in diameter, in which the extent of random disorder is controlled simply by varying the concentration of the particle inclusions, and (ii) low concentration polymer network.

In this presentation, I will be describing our recent results on the LC-NP hybrids of different classes varying in size, shape, anisotropy and the resulting properties.Specifically, the enhancement of the Frank elastic constant, anisotropic electrical conductivity and the permittivity will be discussed. The second type of hybrid is the soft gel formed by particle driven hydrogen-bonding systems, in which a global organo-gel environment and an enhanced local disorder coexist. These features affect the static as well as dynamic properties, including those stimulated by actinic light. The surprising result of an imposed insulating network enhancing the electrical conductivity of a system will also be discussed. Influence of a liquid crystal as a minority component governing the structure in a binary system with a plastic crystal formed by a long chain alkane will be highlighted.

Integral equation theory for two-dimensional Gay-Berne fluid

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We have solved the Percus Yevick (PY) equation for a fluid interacting via the Gay Berne (12-6) pair potential in two dimensions for three length-to-breadth ratios ($x_0 = 3, 3.5, 4$). The correlation functions are expanded in a set of orthogonal functions. PY results have been used in density functional theory (DFT) to locate the freezing transitions of these fluids. We have examined the variation of freezing parameters for the isotropic-nematic transition at two reduced temperatures 1.0 and 2.0. Weak first order transition is found within the version of DFT used at scaled temperature T^{*} =1.0 and 2.0 at all x_0 . Compressibility pressure values are also determined.

Anisotropic Supramolecular Gels: Energy Efficient Smart Materials

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Anisotropic supramolecular gels¹ obtained by incorporating low molecular weight organogelators in a liquid crystalline medium form an important class of physical gels owing to their possible impact in the area of low energy electrical and electro-optic devices. The gels, while retaining the inherent anisotropic properties of liquid crystals (LCs) and the thermo-reversibility of physical gels, have an added advantage of being mechanically robust. The talk presents an overview of recent results obtained from the extensive experimental investigations on anisotropic gels with nematic LC as the host medium. Interesting gelation induced effects such as faster electro-optic response, reduced threshold voltage, enhanced Frank elastic constants, stable nanoparticle dispersions, and high electrical conductivity will be discussed. These novel materials have potential usage in a variety of technological applications such as display devices, actuators, molecular wires etc.

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Localized electroconvection deep in the Freedericksz state of a twisted nematic liquid crystal

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The random evolution of localized structures within an initially homogeneous medium is a characteristic nonlinear phenomenon that occurs in a rich variety of physical, chemical and biological dissipative systems under diverse driving mechanisms [1]. In nematic electro convection in planar cells, such structures, in view of their dynamic nature and slender appearance, are referred to as worms [2]. This study concerns the novel localized periodic structures that evolve deep in the quasi homeotropic Freedericksz state of a 90°-twisted bent mesogen having positive dielectric and conductivity anisotropies. Reverse twisted nematic domains that form in heating and cooling runs are nondegenerate, exhibiting slightly different Freedericksz thresholds. A field induced transformation occurs between the two domains so that eventually the lower threshold state nearly fills the entire cell. However, the state with the initially unfavorable twist-sense reenters in high fields to dynamically coexist with the other state. Localized electro convection observed in high fields manifests in various forms depending on the electrical parameters. Apart from the well-known open-ended worms, we see (i) ring-like dynamic worms, which are essentially metastable electroconvecting walls disappearing via pin cement, (ii) polarity sensitive, large-wavenumber striped patterns forming near the substrates, (ii) circular objects filled with radially travelling waves, and (iv) directed fingerlike branching of disclination loops at the substrates, leading to quasiperiodic labyrinthine patterns with the wave vector along either of the substrate directors.

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Synchronization of conformational chirality in mixtures of achiral bent-core molecules

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Molecular conformational chirality has been proposed as a possible driving force for chiral symmetry breaking in fluids composed of achiral molecules, with deracemization being initiated by segregation of enantiomeric conformers. Using binary mixtures of liquid crystals made of achiral bent-core molecules, we show that enantiomeric excess depends on chirality synchronization between conformers. This is manifested by the formation of two types of lamellar dark mesophases viz. the dark enantiomeric phase characterized by only one sense of chirality and the dark conglomerate phase composed of homochiral domains with opposite handedness. The severity of layer deformation in the dark phases, resulting from the frustration caused by the packing of chiral conformers within the layers is also found to depend on concentration. Electro-optic and dielectric responses reflect the layer deformation and the compactness of the sponge like layer structure and hence the efficiency of conformer packing. The severity of layer deformation has been monitored by visualizing the layer profiles using SEM. This type of study can contribute to the understanding of selective homochirality at the molecular level in achiral systems.

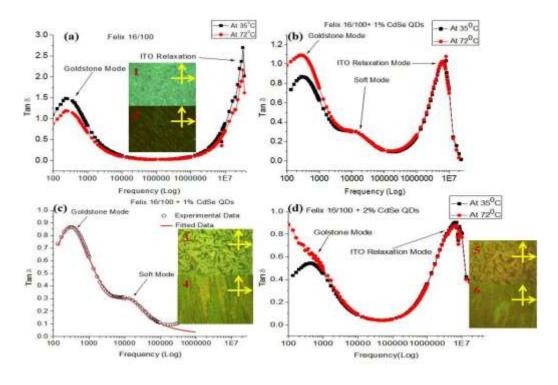
Role of Quantum dots in Liquid crystals and their applications

Rajiv Manohar

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The properties of mesogenic materials may be tuned using nanoaterials. These nanomaterials may be carbon nanotubes, nanoparticles and quantum dots. We have explored the dispersion of these quantum dots with liquid crystals (LCs) and found some interesting results which are very important from fundamental point of view and also for their applicability in devices. During our experimental studies on various LCs doped with quantum dots we have observed concentration dependence of transition temperature, dielectric parameters, spontaneous polarization and rotational viscosity etc. In the present talk various aspects of these dielectric and electro-optical properties will be discussed for doped LCs as a function of temperature, frequency and the dopent concentration in the light of guest host interactions. Several new aspects which came into the light (like CdSe quantum dots induced soft mode) and few new concepts arising out of experimental results will also be discussed. The talk will also cover the changes taking place in the vital parameters due to doping of quantum dots and their probable impact on future applications of LCs.



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Twist-Bend Nematic phase- Behaviour of permittivity and Elastic Constants at atmospheric and at high pressure Srividhya Parthasarathi, <u>D.S. Shankar Rao</u>, Nani Babu Palakurthy, C.V. Yelamaggad and S. Krishna Prasad

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We describe permittivity and Frank elastic constant measurements in the nematic phase of a binary system exhibiting a transition between the nematic (N) and the recently discovered twist-bend nematic (N_{TB}) phase at atmospheric as well as elevated pressures. Among the salient features observed at atmospheric pressure are (i) the existence of the N_{TB} phase even when the system is loaded with a high concentration of a rod-like component, (ii) Clear signature in permittivity at the $N-N_{TB}$ transition, (iii) Bend elastic constant is lower than splay over a large phase space. Application of pressure initially decreases the magnitude ε_{\perp} (permittivity perpendicular to the nematic director) and with further increase in pressure exhibits an increase in the value, feature similar to that obtained at room pressure when the RLN is doped at a high concentration. The dielectric anisotropy exhibits a trend reversal with temperature, the extent of which is affected at high pressures. Another salient feature is that application of pressure enhances bend elastic constant by a large factor of 5, whereas the splay constant (K₁₁) exhibits a much smaller change of only 70%. We propose that all these features can be understood in terms of the relative population of the more energetic horseshoe, and lower energy extended conformer adopted by the CB7CB molecule an argument validated by Xray diffraction experiment.

Synthesis and characterization of oxadiazole liquid crystals with R-(-)-2-butanol terminal unit Mahabaleshwara Subrao¹, <u>Maddasani Srinivasulu¹</u>, Pallavajhula Venkata Chalapathi², Sripada Venkata Subrahmanyam² and Potukuchi D.M.²

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Unsymmetrically substituted 1,2,4-oxadiazoles with alkylbenzoates at C-3 and a biphenyl ester at C-5 are synthesized and characterized. 4-bromo-benzoic acid is esterified with a chiral (R)-(-)-2-butanol and is converted into the corresponding boronic ester. This boronic ester is treated with the 4-bromophenyl oxadiazoles to give the biphenyl substituted oxadiazoles under Suzuki coupling reaction conditions. All the compounds are characterized by ¹H NMR, FTIR and Elemental Analyses. The mesomorphism is characterized by POM and the thermodynamics of phase transitions are determined by DSC. The compounds are found to exhibit SmA and SmC* phases. The spontaneous polarization exhibited by these compounds is studied by field reversal method. The intermediate compounds of the series are found to exhibit higher mesomorphic thermal ranges.

Nematic director deformations and defect around low symmetric colloidal particles of spiral shape <u>Manoj Bhushan Pandey¹</u> Bohdan Senyuk², Quinkun Liu² and Ivan I. Smalyukh²

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Liquid crystals (LCs) are promising host media for reconfigurable self-assembly of microsized colloidal particles¹. Particles dispersed into LCs induce defects and deformations of a nematic director field $\mathbf{n}(\mathbf{r})$, forming nematic colloidal particles with the inclusions typically surrounded by coronas of elastic distortions of the molecular alignment propagating to large distances, which can be analyzed in terms of elastic multipoles in analogy to their electrostatic counterparts¹⁻³. One of the central experimental efforts in nematic LCs colloids research aims to explore how the interplay between the geometry of particles along with the accompanying nematic director deformations and defects around them can provide a means of guiding particle self-assembly and controlling the structure of particle-induced defects.

In the present work, we study properties of elastic multipoles created in nematic LCs by lowsymmetry colloidal particles with complex geometrical shape of spirals⁴. We show that these spiral-shaped particles can induce director distortions and defect configurations with nonchiral or chiral symmetry, which are controlled by varying surface functionalization of particles to provide tangential or homeotropic boundary conditions for the nematic director. These nematic colloidal particles also exhibit both stable and metastable orientational states with respect to the homogeneous far-field director and induce a large number of configurations featuring both singular and solitonic nonsingular defects accompanying them, which can result in unusual forms of colloidal self-assembly.

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Oral Lectures

Pseudo-Polar Tilted Smectic Phases of Bent Rod-like Molecules

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Bent rod-like molecules are now known to exhibit some fascinating liquid crystalline phases between their solid crystal and isotropic liquid states. Some of these liquid crystalline phases are quite different from that exhibited by rod-like or disc-like molecules. The simple bent structures of the molecules introduce shape polarity and biaxiality in their molecular structures. The symmetrically bent banana shaped molecules can induce spontaneous breaking of chiral symmetry and switchable layer polarization in their smectic phases. Here we present experimental and theoretical studies on asymmetrically bent hockey stick shaped rod-like molecules exhibiting two new smectic phases1. The packing of these bent-core hockey stick shaped molecules in the layers leads to a pseudo-polar order in these tilted smectic phases. An anticlinic SmC A type stacking of the pseudo-polar layers is observed in the higher temperature smectic phase, while in the lower temperature phase the difference in the azimuthal angles of the tilt directions in successive layers is between zero and π with a randomized tilt organization between the successive layers. The randomness arises due to the sign degeneracy of the azimuthal angle difference of the tilt directions in successive layers. Both of these smectic phases show electro-optic response which can be exploited for potential applications.

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Dilatational rheology studies on thin film of ferroelectric copolymer at air-water interface Chandan Kumar¹ and P. Viswanath¹

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Poly (vinylidene fluoride tri fluoroethylene), P (VDF-TrFE) (70:30) is an important member of ferro and piezo electric class of polymers [1]. The polar phases of these polymers are particularly interesting due to its diverse applications. We have investigated the dilatational rheological response of the Langmuir film of polymer, P (VDF-TrFE) using oscillatory compression technique at different surface pressures, temperatures and frequencies. The sinusoidal stress and the strain curves of the polymer monolayer were analysed using Fourier transform method. The Fourier transform analysis of the rheological response of the polymer film shows the presence of higher harmonics in addition to the dominant fundamental mode. Using the amplitudes and phases of the fundamental mode, we have determined the viscoelastic modulus of the polymeric film. Strain sweep studies show typical behaviour characteristic of semi-crystalline polymer. Frequency sweep studies show a crossover behaviour which is sensitive to temperature. Further, the temperature dependence study of the elastic moduli show a pronounced discontinuity at 298 K suggesting a phase transition [2].

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Current Sensing Atomic Force Microscopy Studies on Langmuir Blodgett Film of a polymeric liquid crystal <u>Bharat Kumar¹</u>, Gayathri H. N.², K. A. Suresh², H. K. Bisoyi³, Sandeep Kumar³

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The monolayer film of a novel liquid crystalline polymer derived from 2,6-dihydroxy-3,7,10,11-tetraalkoxy-triphenylene (PHAT) was studied using current sensing atomic force microscopy (CSAFM). The monolayer of PHAT was formed on a conducting gold substrate by the Langmuir–Blodgett (LB) technique. The gold substrate–PHAT monolayer–cantilever tip of CSAFM forms a metal–insulator–metal (M–I–M) junction. The analysis of the nonlinear I–V characteristics of the M–I–M junction showed that the mechanism of charge transport in the liquid crystalline polymer monolayer is by direct tunneling. Our studies help in understanding the effect of polymerization of molecules containing triphenylene moieties on the electrical properties of M-I-M junctions formed by such molecules.

Asymmetrical 1, 3, 4-oxadiazole bent core liquid crystals possessing lateral methoxy group: Nematic phase Manoj Kumar Paul, Sandip Kumar Saha

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In recent years, the nematic phases of bent core mesogens (BCMs) have received considerable research attention because of their special properties such as biaxiality, gaint flexo-electricity, negative bent -splay anisotropy, ferro-electric switching etc. and potential for fast display device applications due to much faster switching than presently used nematic phases in display devices [1]. The central bent-core unit, side arms, their linking group, polar and non-polar substitution in the central bent core unit or side arm play significant role in the formation of bent-core nematic liquid crystals [2]. In recent years, heterocyclic 2, 5disubstituted 1, 3, 4-oxadiazole derivatives are widely used as bent core unit in the BCMs [3]. Moreover, the electron deficient nature of 2,5-disubstututed 1,3,4-oxadiazole moiety lead to luminescent materials which is one of fascinating recent topic of material research. Therefore, new asymmetrical 1, 3, 4-oxadiazole bent core liquid crystals possessing lateral methoxy group have been designed and synthesized. The phase transition temperatures and characterization of phase behavior of the compound was investigated by using polarizing optical microscope and differential scanning calorimetry. The compounds exhibited nematic phase at ambient temperature. The photophysical properties of the compounds were explored using the UV-visible and fluorescence techniques in solution and thin film. The compounds are fluorescent in nature.

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Functionalized triphenylene: Synthesis and Thermal Properties

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We present the exclusive and simple synthesis procedure for the preparation of mono- and difunctionalized triphenylene. The metal mediated oxidative coupling of 2-halo(alkoxy)benzene with tetra(alkoxy)biphenyl by FeCl₃ or MoCl₅ as oxidizing reagent yields monofunctionalized triphenylene. Further, Reaction of hexa(alkoxy)triphenylene with nitric acid (>90%) yielded hexa(alkoxy)-1,5-dinitrotriphenylene together with the regioisomer hexa(alkoxy)-1,8-dinitrotriphenylene. The molecular structure of functionalized triphenylene was confirmed by spectroscopic and spectrometric analysis. The thermal properties were investigated by polarizing optical microscopy, differential scanning calorimeter and X-ray diffraction studies (XRD). The functionalized triphenylene exhibits the columnar phase. The effect of functionalizing of pentakis (alkoxy) triphenylenes or hexa (alkoxy) triphenylene will be discussed.

Stability of DNA molecule in crowded environment Navin Singh

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The thermal melting of double stranded DNA (dsDNA) is studied in the crowded environment. The crowded sites are selected randomly along the chain and effect of their presence on melting behavior of the molecule is studied. With suitable modifications in a statistical model we calculate the melting profile and the melting probabilities of the chain. Through the density plots we investigate the opening of the DNA molecule in the presence of molecular crowders.

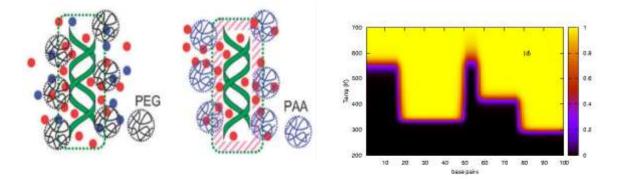


Figure: (a) The DNA in cell is surrounded by biomolecules. (b) The density plot that shows the opening of DNA molecule in thermal ensemble.

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Autonomous motion of deformable objects Snigdha Thakur

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Self-propelled motion involving conversion of chemical energy to mechanical energy internally is widespread in nature. Examples include biological motors which play essential roles in the transport and synthesis biochemicals in the cytoplasm and in cell motility [1, 2]. In addition to these biochemical motors, synthetic molecular motors have been designed that use chemical, light, or other energy sources to perform directed motion. Model for one such class of synthetic motors, where the motion does not rely on the conformational changewill be discussed [3]. This class of motors includes electrochemically synthe-sized striped bimetallic nanorods and synthetic catalytic molecules tethered to inactive particles. We also probe the collective behaviour of such motors.

The chemo-mechanical propulsion is not limited to particle-like elements, rather there are many instances where such conversion occurs on filaments [4]. The the dynamics of such active semi-exible _lament will be discussed. We show that the filament exhibits three distinct type of motion, namely, translational, snaking and rotation: as the rigidity of the filament decreases. Further, the autonomous propulsion of a chemically powered vesicle will be discussed.

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Synthesis and Computational studies of Liquid crystal with nanoparticles

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Synthesis of liquid crystal with nanoparticles has driven device technology altering the physical and electro optical properties. Cholesteryl stereate [1] exhibiting nematic liquid crystalline nature is conjugated with four nano particles viz Iron, Zinc, Alluminium and Copper to form a complex. Experimental studies were carried for particle size confirmation with XRD technique. Studies performed with FTIR and Raman studies [2] were absolutely correlated. Computational studies were carried Hartree Fock method with 6-31G* basis set for individual and conjugated for optimized structures. The frequency assignments computed were in good agreement experimental studies. The liquid crystalline nature is strengthened in aluminum and copper nano particles (<50nm) than with others (>50<100nm).Spectroscopic properties were realized to explain the enhanced activity of spin-spin interactions with reduced energy gap. The performed studies with these particles may have good application in development of optical materials suitable for display technology.

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Scientific and technological development of liquid crystal based optical memory Jai Prakash¹ and Ashok M. Biradar²

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Liquid crystals (LCs) are unique, self-assembled, dynamic functional soft materials, which possess high degree of anisotropy (shape, dielectric, and optical), order and mobility at molecular, supramolecular and macroscopic levels [1, 2]. The memory behaviour in LCs has made very significant headway over the past three decades since their discovery in nematic type LCs. The memory element formed by numerous LCs have been protected as patents, a few have been commercialized too, as compensation to non-volatile memory devices, memory used in personal computers and digital cameras, and futuristic low cost, large area, high speed, high density memory needed for advance computers and digital electronics. Short and long duration memory behaviour for industrial applications have been obtained from the several LC materials and a liquid-crystal memory with interesting features and applications has been demonstrated by using numerous LCs. However, considerable challenges still exist in searching for highly efficient, stable, and long-lifespan materials and methods so that the development of useful memory devices could be possible.

Here, we review the scientific and technological approach of fascinating applications of LCs based memory. We cover the introduction, development status, novel designing and engineering principles, and parameters affecting LC memory. We also deal with the facts that how the amalgamation of LCs with emerging field of nanotechnology could bring significant change/improvement in memory effect in the former and application of LC memory as the active component for futuristic and interesting memory devices.

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CdSe Quantum dot dispersed FLC matrix: Dimensional correlation on the physical properties of composite <u>Kamal Kumar Pandey¹</u>, D. P. Singh,² A. Daoudi,² S. Kumar,³ and R. Manohar⁴

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Octadecylamine capped cadmium selenide quantum dots (CdSe QDs) having two different diameter (2.4 and 3.5 nm) were dispersed in FLC matrix. The effect of dimensional correlation of QDs with that of the FLC molecular length was investigated using electro-optical, optical microscopic and phase transitional techniques. If the size of QDs is comparable or lesser than that of the molecular length of FLC molecule, they don't perturb the helical geometry of FLC structure. The primary and secondary order parameters of FLC also remain almost same even after the dispersion of dopant in small concentrations. Electro-optic response of composites becomes faster whereas a small change in SmC*-N* and N*-I phase transition temperatures were observed. Such composites can be utilized in faster electro-optical devices.

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Tuning phase retardation behaviour of nematic liquid crystal using quantum dot

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Nematic liquid crystals (NLCs) are the widely used LC in the production and fabrication of LC displays worldwide. Liquid crystals are anisotropic materials; the change in director gives rise to change in the values of different physical parameters. Therefore it is necessary to align the LC molecules more effectively to use them in LC devices. A study of birefringence and other parameters in NLC and its variation with doping of QDs has been presented. The study shows change in NLC ordering after addition of QDs. The observed values of birefringence in QD doped NLC system has been attributed to change in alignment introduced by QDs. The transform in order of NLC system has also been explained by schematic illustrations for pristine and QD doped NLC system. Study of relative permittivity has also revealed the ordering effect in QD dispersed NLC system.

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Synthesis and thermally stable luminescence of $SrGd_{2(1-x)}Eu_{2x}O_4$ samples for lighting and display applications Jyoti Singh¹ and Jairam Manam¹

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Nowadays, rare-earth (RE) doped binary oxides having general formula ARE_2O_4 (where, A= alkaline earth metals, RE= rare-earth elements) optical materials are receiving extensive interest because of their favourable applications towards the development of display devices such as field-emission displays (FED), plasma display panels (PDP) and white light-emitting diodes (W-LED) [1].

In this context, $SrGd_2O_4$ (strontium gadolinium oxide) has chosen as a host lattice synthesized by combustion method and Eu³⁺ ions used as a dopant in order to yield strong red emissions. The structural and optical properties of prepared phosphors are measured by XRD, FTIR, FESEM, PL and UV-Vis characterizations. The XRD results revealed the orthorhombic $SrGd_2O_4$ phosphor with space group Pnam (62) appears as the dominant phase [2]. The main structural entities are confirmed by FTIR studies. FESEM studies revealed the agglomerated rod-like morphology with average size 0.3-3 µm.

The photoluminescence (PL) excitation and emission spectra show the characteristic emission peaks of Eu³⁺ due to its presence in the host-lattice. The most intense peaks of Eu³⁺ were obtained at 615 nm and 595 nm which correspond to ${}^{5}D_{0} \rightarrow {}^{7}F_{2}$ and ${}^{7}F_{1}$ transition respectively. To know the thermal stable behaviour of present system, temperature dependent PL is performed and samples showed adequate thermal stability even at 200 °C. Photometric characterization and elevated physical and chemical durability indicated the suitability of SrGd₂O₄:Eu³⁺ phosphor for pure red emission in white LEDs and other display applications.

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Liquid Crystals confined to toroidal droplets: A Monte Carlo Study

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Liquid crystals confined to restricted geometries like spherical and cylindrical geometries have been observed to show interesting defect textures in the nematic phase. In the recent studies bulk order behaviour of nematic liquid crystals were also studied to observe the effect of temperature vis-à-vis surface induced anchoring in such confined geometries [1]. Very recently liquid crystals confined to toroidal droplets with one or more handles are stabilized experimentally [2] giving rise to interesting director configurations in nematic phase. The focus of the present work is to investigate the effect of temperature and surface induced anchoring on the bulk ordering of liquid crystal molecules in such restricted geometries, particularly near the nematic-isotropic (NI) phase transition using Monte Carlo based simulations. Further, the defect textures in the nematic phase are studied under the influence of both homeotropic as well as planar surface anchoring.

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Nanoparticle dispersion in liquid crystals <u>Satya Prakash Yadav¹</u>, Rajiv Manohar², Shri Singh¹

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Dispersion of Nanoparticles in liquid crystalline materials has attracted a great deal of interest during past years, both experimentally and theoretically. The impact of dispersion of nanoparticles has resulted in enhancement of the performance of LC based devices.

In this report, we study how nanoparticles dispersion in liquid crystalline materials influences the various properties of liquid crystals. Broadband dielectric spectroscopy (100 Hz – 40MHz) has been performed as a function of temperature with $7\Box$ m thick cell. Different parameters such as Relaxation time, Dielectric permittivity, Electric Conductivit etc. have been measured. Electro optical parameters show enhancement with the dispersion of nanoparticles.

Defect-induced microstructures of spherical microparticles and their effect on the rheological properties of 8CB liquid crystal

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We report detailed rheological studies on the liquid-crystal-colloids prepared by dispersing silica microparticles with homeotropic surface anchoring in 8CB liquid crystal. The apparent yield-stress increases in both the nematic (N) and smectic-A (SmA) phases with increasing volume fraction of particle. The rheomicroscopy studies reveal the dynamics of the dipolar colloidal chains under shear. An unusual behavior in the shear-rate dependent apparent viscosity is observed near the N-SmA transition. The critical strain amplitude (γ_c) in the SmA phase decreases significantly with the increasing volume fraction of particles. The frequency-dependent storage modulus of the SmA phase shows a power-law behavior ($G'(\omega) \omega^{\alpha}$) with exponent ' α ' that depends on the particle density and the loss modulus (($G''(\omega)$) exhibits a shallow minimum. Our study shows the effect of shear on the defect-induced microstructures and their contribution on the rheological properties of 8CB liquid crystal.

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Orientational order and cone angle of twist-bend nematic phase in the mixtures of achiral cyanobiphenyl bimesogens <u>Gautam Singh^{1,2}</u>, D. M. Agra-Kooijman², M. R. Fisch³, M. R. Vengatesan⁴, Jang-Kun Song⁴, and Satyendra Kumar^{2,5}

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The twist-bend nematic (N_{TB}) phase possessing heliconical structure¹⁻² forms at a lower temperature than the regular nematic (N) phase in achiral cyanobiphenyl (CB) bimesogens with odd number of -CH2- segments linking the two CB moieties, e.g., molecules CB $(CH_2)_n$ CB, with odd value of n. Even homologues of this series do not form the N_{TB} phase³. The precise phase structure of the N_{TB} phase and phase transition between the two nematic phases in these and other systems are intriguing and remain under extensive investigations. We studied the single component and mixtures of odd (n = 7) and even (n = 6) homologues using polarizing optical microscopy and high-resolution x-ray scattering to gain deeper insight into N_{TB} phase. Thermal evolution of the orientational order parameters $\langle P_2(\cos\theta) \rangle$, $\langle P_4(\cos\theta) \rangle$, and $\langle P_6(\cos\theta) \rangle$ in both nematic phases were determined using x-ray scattering. Both $\langle P_2 \rangle$ and $\langle P_4 \rangle$ were found to increase with decreasing temperature in N phase, as expected. The value of $\langle P_6 \rangle$ remains near zero at all temperatures in both phases. However, both $\langle P_2 \rangle$ and $\langle P_4 \rangle$ decreases in the N_{TB} phase. While $\langle P_2 \rangle$ remains positive, $\langle P_4 \rangle$ becomes negative in N_{TB} phase far below the transition. This provides the first direct evidence of the heliconical arrangement of bimesogens having the volcano-like orientational distribution function (ODF). The temperature dependence of heliconical tilt angle (α) estimated from the ODF in the N_{TB} phase reveals a weakly first order $N-N_{TB}$ phase transition in all samples. The effect of temperature and concentration on macroscopically averaged tilt angle, pitch and stripe width measured from rope-like optical textures in homogenously aligned cells will be discussed. [†]Supported by the Office of Basic Energy Sciences, DOE, grant # DE-SC0001412.

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Hair Cleaning in a Clean Way: Natural versus Synthetic Shampoos

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Hair care has been essential to mankind since ancient times. The market today is replete with synthetic hair care products which have pushed natural materials to the background. These natural materials, obtained from plants, are bio-degradable and non-toxic. In a bid to investigate natural products, we studied the surface tension, foaming and relevant parameters of natural surfactants extracted from plants traditionally used in hair care, namely Shikakai (*Acacia concinna*) and Seto Siris (*Albizia procera*) in aqueous solution. As a reference, a synthetic shampoo has also been studied.

Shikakai is acid balanced and demonstrates very prominent surface tension reduction, high foaming, wetting and cleaning, showing it to be a potential candidate for good hair care. Seto Siris is mildly alkaline, exhibits good surface tension reduction possess high viscosity and conductivity and shows good dirt dispersion, making it a decent natural cleansing agent. Qualitative measurement of cleaning properties and subsequent comparison with commercial shampoo shows that both plants have a large potential in providing non-toxic natural hair care. Preliminary characterization of the natural surfactant (saponin) obtained from Shikakai using UV-Vis and FTIR spectroscopy is underway.

Keywords: Saponin, Foam formation, FTIR, Surface tension.

Rod –disc oligomeric liquid crystal based on 4cyanobiphenyl and truxene core Indu Bala¹ and Santanu Kumar Pal¹

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The majority of discotic liquid crystals (DLCs) are derived from polycyclic aromatic cores such as, triphenylene, anthraquinone, pthalocyanine and hexabenzocoronenes *etc.* However, the numbers of reported truxene DLCs are limited because of the difficulties of preparation and purification. In 1981, Destrade and co-workers first studied the truxene in discotic liquid crystals by preparing the hexaesters of truxene showing inverted nematic-columnar phase sequence. Truxene derivatives are among the earliest discovered discogens. Truxene based compounds are attractive for many applications such as optoelectronics, photovoltaics, polymers, dyes, semiconductors, polymeric light emitting devices *etc.* because of it being an electron rich system, C3 symmetrical structure, good fluorescence capacity, extraordinary thermal stability and its electronic properties.

One of the most active areas of research in liquid crystal science in recent years has been the search for the elusive biaxial nematic phase. In these simulations an attractive interaction is required between the rods and discs to prevent phase separation into two uniaxial nematic phases and in real system phase separation does indeed occur. To overcome this difficulty a number of authors have attached rod-like and disc-like units *via* flexible alkyl spacers. In these molecular systems a single rod and disc have been interconnected and such dimers have been the subject of the computer simulation study. Discotic nematic of truxene core using ester functionality is known in which re-entrant columnar phase occurs, Herein, we made an attempt to make a discotic nematic of truxene and got success in which only pure nematic phase is there and no re-entrant columnar phase came. We have synthesized truxene derivative in which six rod-like 4-cyanobiphenyl moieties are attached to a central truxene core *via* flexible alkyl spacers. The mesophase was confirmed by DSC, POM and XRD.

Synthesis and Characterization of sol-gel prepared Al doped ZnO thin films

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Zinc oxide (ZnO) is a wide band gap (3.36 eV) semiconducting material¹. Al doped ZnO thin film is a promising candidate for Transparent Conducting Oxide (TCO) applications². We have prepared ZnO thin film by sol-gel spin coating technique. Aluminium chloride was used as precursor for Al doping. Structural, optical and electrical characterizations of the synthesized films were carried out. Highlights of the work include:

- X-ray diffraction of Al doped ZnO films revealed Hexagonal wurtzite phase.
- Al doping was confirmed using energy dispersive scattering.
- Narrowing in optical band gap of film was observed.
- Low temperature resistance measurement showed semiconducting behavior.

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Self-Organized 3D quasicrystals in nematic liquid crystals Sai Praneeth Madduri¹, Jayasri Dontabhaktuni¹

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Nematic liquid crystals have the remarkable property of assembling the colloidal particles into structures of various symmetries based on their orientational ordering. Two-dimensional colloidal tilings were assembled by shape-tuning of polygonal colloidal platelets in nematic liquid crystals. It is found that depending on the shape of the platelets the colloids assemble themselves either into quadrupolar or dipolar symmetries [1]. We had shown recently for the first time using numerical simulations that on additional symmetry-breaking one can also assemble quasicrystalline tilings [2]. This additional symmetry breaking can be achieved either by tuning the surface anchoring on the platelets or by introducing particles with truncated edges on one side of the mid-plane passing through them [3]. In the present work we extend this further to assemble the platelets in three dimensions with quasi-crystalline symmetries for the very first time.

Surface anchoring on the pentagonal platelets is tuned to introduce symmetry-breaking about two perpendicular planes passing through the platelets. We demonstrate for the first time that it can give rise to approximants of icosahedral symmetries. In experiments one can also achieve this by introducing particles with tapered edges on one side of two perpendicular planes passing through the platelets. Such tunable quasicrystalline structures in 3D are believed to be good candidates for applications as photonic crystals.

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Nano crystalline rare earth doped phosphors for lighting, display and forensic

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We will discuss some of our recent experimental results based on the nanocrystalline rare earth doped upconverting phosphors for lighting, display and forensic applications. The nanocrystalline rare earth doped upconverting phosphors exhibit sharp emission peaks due to its radiative transitions originated from 4f-intra configuration. We show that these nanocrystalline rare earth doped phosphors upon 980 nm laser diode excitation provide multicolour upconversion emission features. Now a day, tunable and non-tunable phosphors are fascinated much more attention among the researchers because of low power consumption for the production of lighting and display devices. The upconversion emission mechanism has been explained via sketching the energy level structure. For green and blue upconversion emission, we choose Er^{3+} and Tm^{3+} ions for doping in different low phonon frequency host lattices. The developed nanocrystalline rare earth doped phosphors have been demonstrated in latent finger mark detection and security ink application.

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Refractive index studies of nematic liquid crystals exhibiting high birefringence

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Liquid-crystalline material research has contributed significantly both to the development of liquid-crystalline display (LCD) technology and also to the better understanding of the phase transitions of soft condensed matter systems. Optical birefringence is considered as the basis of various liquid crystals device applications. Keeping the applicability of these high Δn LCs in mind, we carried out the optical studies on two highly birefringent nematic LCs viz., 4'butylcyclohexyl - 3, 5 - difluoro - 4 - isothiocyanatobiphenyl, 4'- pentylcyclohexyl - 3, 5 difluoro -4 - isothiocyanatobiphenyl. The two LC compounds were found to exhibit fairly high clearing temperatures (135.2 ° C and 196.3 ° C respectively). Measurements of refractive indices of the two compounds were done by using thin prism method with He-Ne laser beam of wavelength 630 nm. Both the compounds are found to display fairly high values of birefringence ($\Delta n \sim 0.3$). Validation of a modified four-parameter model, based on Vuks equation describing the temperature dependence of refractive indices of the two liquid crystals, is also presented in this paper. The model is validated by fitting the experimentally measured values of refractive indices, birefringence and average refractive indices of the two nematic LCs with the theoretical values. The high values of optical birefringence exhibited by these liquid crystals may make them suitable for better device applications.

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Effect of counterions on the binding affinity of alkali metal ions with phospholipid membranes Pabitra Maity¹ and Sanat Karmakar¹

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The effect of alkali metal ions with negatively charged phospholipid membrane is important in order to understand the structure and functions of biological membranes at physiological condition. We have systematically investigated the effect of counterions on the binding affinity of Na⁺ ions with phospholipid membranes using dynamic light scattering, zeta potential and isothermal titration calorimetry. As a model system, we have prepared large unilamellar vesicles (LUV) using extrusion techniques and size distributions have been confirmed from dynamic light scattering. Zeta potential obtained from electrophoretic mobility was used to determine the binding affinity of various monovalent cations to the membranes. The concept of electrostatic double layer, as described by the Gouy Chapman theory, has been employed to estimate the intrinsic binding constant of Na⁺ with the membranes. Binding constant estimated from the zeta potential was in agreement with that obtained from the isothermal titration calorimetry study. The reasonable and consistent binding constant has been obtained at 10 to 100 mM ion concentrations. However, at high ionic concentrations (> 100 mM), we were not able to estimate intrinsic binding constant of ions. This might be due to the fact that at higher ionic concentrations, the screening effect is more significant over the binding phenomenon. Therefore, we suggest that Gouy Chapman theory can be applied to intermediate salt concentrations only. The effect of counterions on the binding affinity of Na⁺ follows the order I > Br > CI for neutral DOPC membranes. However, for negatively charged membranes, the order is Br > I > Cl. Several types of fluorescence experiment suggest that among all anions I adsorbes and penetrates significantly into the membranes. Our study provides an important insight into the ion-membranes interaction.

Synthesis, Characterisation of citrate capped gold/ZnO nanoparticles and its effect on liquid crystals – Optical Studies

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In the present paper synthesis and characterization are carried on citrate capped Gold (Au) nanoparticles and ZnO nanoparticles dispersed in Liquid Crystalline p-n-Hexyloxy cyanobiphenyl (6OCB) compound. We report Citrate capped Au nanoparticles are synthesized by chemical reduction method and ZnO nanoparticles are synthesized by Autoclave method which are emerging materials that have a broad range of applications and dramatically effects the birefringence properties of 6OCB when dispersion with low concentration. The Polarizing Microscopy (POM), Differential Scanning Calorimeter (DSC) technique are used to measure the phase transition temperatures. Further characterizations are done by various spectroscopic techniques like X-ray Diffraction spectrometric studies (XRD), Scanning Electron Microscopy studies (SEM), Ultra Violet Visible (UV) spectroscopy, Fourier Transform Infra-Red Spectroscopy (FTIR) and Digital spectrometer. Textural determinations of the synthesized compounds are recorded by using POM connected with a hot stage and camera. The result shows that the dispersion of citrate capped Au and ZnO nanoparticles in 6OCB exhibits nematic phase as same as the pure 6OCB with reduced clearing temperature as expected and the nematic thermal range slightly increases. Further, the order parameter is estimated from birefringence anisotropy data using a method developed by Kuczynski etal without considering any internal field model to liquid crystaline molecules and with dispersed citrate capped Au/ZnO nanoparticles. It is found that the birefringence anisotropy as well as orientational order parameter of 6OCB increases with dispersed citrate capped Au and ZnO nanoparticles.

Keywords: Synthesis, polarizing optical microscope (POM), differential scanning calorimeter (DSC), Nano dispersion, X-ray diffraction (XRD), scanning electron microscopy (SEM).

First order reversal curves of ferroelectric liquid crystal (SmC*)

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First order reversal curve (FORC) [1-3] method has been proved as a powerful and practical method of describing the hysteretic and polarization switching processes of ferroic materials, particularly ferromagnetic and ferroelectric with bimodal distribution of coercivities. This method originated in identification procedures for the classical Preisach model and consequently often the FORC distribution is interpreted as a slightly distorted Preisach distribution. FORC method has been used to characterize the domain switching process in ferroelectric liquid crystal (SmC*) [4]. It is interesting as the origin of ferroelectricity in liquid crystalline chiral smectic phase is notably different from that of other solid state ferroelectric materials. Theoretical background of FORC diagram, based on the Preisach model, experimental method and analysis process have also been discussed in detials. The FORC diagrams showing reversible and irreversible contributions to the polarization can clearly be separated as the characteristic of proper ferroelectric materials.

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Gradual growth of ferroelectric mesophase under geometrical confinement in core/shell quantum dot-ferroelectric liquid crystal composite and their ultra-fast electro-optical response for display

application

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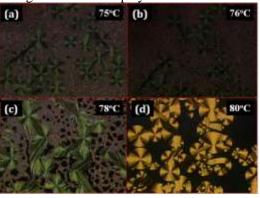
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Cd_{0.15}Zn_{0.85}S/ZnS core/shell quantum dots (CSQDs) of 8.5 nm in diameter were prepared and dispersed in ferroelectric mesophase into different concentrations. Gradual growth of ferroelectric liquid crystal (CSQD-FLC) composite. The mesomorphic properties of composites were studied by X-ray diffraction, UV-visible absorbance and optical texture analysis. The change in geometry evinces the new structure-property correlation in CSQD-FLC composite. The reduction in polarization and ultra-fast electro-optical (E-O) response of composites are the fascinating features for displays.



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Ethylenedioxythiophene: Novel central unit for bent-core liquid crystals

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We have discovered that Ethylenedioxythiophene (EDOT) can be used as a central unit for the synthesis of bent-core liquid crystals (BC LCs). Four series of compounds include three ring and five ring compounds were prepared from EDOT. The mesophase behaviour of all the compounds was characterized using a combination of polarizing optical microscopy, differential scanning calorimetry and X-ray diffraction measurements. EDOT-based threering compounds with acetylene linkage were found to be nonliquid crystalline, while all the four derivatives of five-ring series with acetylene linkage, including a branched alkoxy chain derivative, display enantiotropic nematic phase over wide temperature range. EDOT bearing three-ring Schiff base bent-core compounds are non-mesomorphic but all the Schiff bases containing five-ring exhibit enantiotropic mesophase behaviour. The higher homologues exhibit only N phase. The bent angle of these compounds is about $153^0 - 155^0$, which falls in between typical rod-like and banana liquid crystals¹⁻⁴. The detailed XRD investigations of all the mesogens corroborate the presence of nematic phase and Smc phase.



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s-Triazine - Based Functional Discotic Liquid Crystals: Synthesis, Mesomorphism and Photoluminescence Bhyranalyar N. Veerabhadraswamy and Channabasaveshwar V. Yelamaggad

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The field of organic electronics is an emerging and vastly developing research area wherein π -conjugated organic materials are used as active components in various electronic devices, such as field effect transistors (FETs), solar photovoltaics (PVs), organic light-emitting diodes (OLEDs), sensors, etc.^[1-8] We have designed and synthesized a new series of C_3 symmetric, π -conjugated molecules derived from electron-accepting s-triazine, appended covalently to electron donating styrylbenzene arms. Examination of the phase transitional properties by several complementary techniques evidences self-assembly into a hexagonal columnar phase, occurring over wide and reasonable thermal ranges. The photophysical properties were studied both in solution and in the fluid/frozen columnar states by UV/Vis absorption and photoluminescence spectroscopy. The emission spectra obtained as a function of the temperature rule out the breaking-up of larger columns and a non-radiative, thermally activated process. A study carried out on thin films of the glassy columnar state, which accounts for conserved fluorescence, defect-free orientation, and freezing ionic species, with the help of atomic force microscopy (AFM) images, suggested a homogeneous granular morphology comprising fibrillar structures. Dissimilarities in the surface morphology and birefringence of thin films of the solid and frozen columnar states were clearly shown by Raman spectroscopy. An electrochemical investigation revealed LUMO energy of -4.0 eV. Thus, the discotic motifs presented herein meet certain criteria of organic materials, which are essential for developing electronic devices.

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Phosphorescent Columnar Hybrid Materials: A Supramolecular Approach <u>Susanta K. Nayak^{1,3}</u>, M. Amela-Cortes¹, M. M. Neidhardt², S. Beardsworth², J.

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Columnar liquid crystals (CLCs) have attracted much attention in materials chemistry after Chandrasekhar discovered discotic benzene hexaalkanoates in 1977¹. These materials are shown to be useful in the design of many devices including photovoltaic solar cells, field effect transistors, one dimensional conductor, and light emitting diodes because of it selforganisation process into columns and self-healing properties². In many cases, non-diskshaped molecules can form columnar mesophases, which were also used to organise small amounts of bulky inorganic components such as gold nanoparticles,³ gold nanorods,⁴ or quantum dots over a wide range.⁵ Addition of new functionalities to CLCs, e.g., phosphorescence, appears then, to be particularly appealing in terms of application prospects but still remains very challenging in terms of liquid crystals phase or emission stability. In this presentation, we show the ternary polyionic inorganic compound $Cs_2Mo_6Br_{14}$ and 18crown-6 ethers bearing two o-terphenyl units have been combined to design phosphorescent columnar liquid crystalline hybrid materials by supramolecular approach. The obtained hostguest complexes are very stable even at high temperatures. Depending on their surrounding atmosphere, these hybrids switch reversibly from a high-to-low luminescence state and show very stable emission intensity up to $140 \,^{\circ}\text{C}^{\circ}$.

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Electrical parameters of room temperature single phase antiferroelectric liquid crystalline material for photonic application

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The antiferroelectric (SmC_a^*) phase of liquid crystal is not only fundamentally interesting but also very attractive for an application point of view such as displays, optical switches and routers, tunable, focus lenses, wavelength selective filters and variables, optical attenuators tunable electrical filters [1]. Electrical response of a room temperature single phase antiferroelectric liquid crystalline material (S)+(1-methylheptyloxycarbonyl)2-fluorophenyl 4'-(3-perfluoropropylmethylnoyloxy prop-1-oxy)biphenyl-4-carboxylate has been investigated.

$$C_{3}F_{7}CH_{2}OC_{3}H_{6}O$$
 $COOC^{*}H$ $C_{6}H_{13}$ (S) CH_{3}

Figure – Molecular structure of (S)+(1-methylheptyloxycarbonyl)2-fluorophenyl 4'-(3-perfluoropropylmethyl noyloxyprop-1-oxy)biphenyl-4-carboxylate.

Dielectric, thermodynamic and texture studies show wide room temperature range (~87°C to < 22°C) antiferroelectric SmC^{*}_a phase exhibits in this material. The electrical parameters have been measured in the frequency range 1 Hz to 35 MHz under planar anchoring conditions of the molecules. The dielectric response of the SmC^{*}_a phase exhibits three relaxation modes due to collective as well as individual molecular process. Its relative permittivity (at 10 kHz) varies from ~ 5.24 at 89.0 °C to 6.11 at 29.0 °C. The ionic conductivity, spontaneous polarization, switching time and critical electric field of the material is also measured.

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Imaging Ellipsometry Studies on Cholesterol and Cholesteryl Esters at Air-Water and Air-Solid Interfaces Arup Sarkar and K. A. Suresh

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Cholesterol and cholesteryl esters are vital components of arterial plaques and cell membranes. We have studied the phases exhibited by Langmuir films of cholesterol and cholesteryl esters at air-water interface using surface manometry, Brewster angle microscopy and imaging ellipsometry. The variation in thickness of the film as a function of area per molecule was measured using imaging ellipsometry simultaneously with surface manometry measurements. We find that cholesteryl laurate forms unstable fluidic bilayer phase which transforms into crystalline bilayer phase with time. We have transferred the films from airwater interface onto hydrophilic silicon substrate by Langmuir-Blodgett technique and studied using imaging ellipsometry and atomic force microscopy. We find that on transferring to silicon substrate films of cholesterol and cholesteryl esters except cholesteryl nonanoate retain the same texture as that at air-water interface. The thickness of a film in a particular phase measured by imaging ellipsometry at air-water interface agrees well with that measured at air-solid interface by imaging ellipsometry and atomic force microscopy.

Use of Liquid Crystal Thermography over Artificial Roughness to Enhance Heat Transfer – A Review Apurba Layek

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The development of liquid crystal (LC) based thermography is relatively inexpensive technique that allows visual determination of both qualitative and quantitative heat transfer and fluid flow information on heated objects placed in forced convection environments. The technique employs cholesteric liquid crystals as the temperature sensing agent. Scientist and engineers are applying liquid crystal thermography for visualizing and measuring surface temperature on a wide variety of engineering applications, such as electronics cooling, gas turbine heat transfer, boiling heat transfer, and fluid temperature measurement. This technique is also applied to get the detailed information of local Nusselt number distribution caused by periodic rib roughness exist in different engineering applications.

The surface modification like applying artificial roughness in the form of rib or groove over heat transferring surface act as turbulent promoter and enhances the heat transfer. Roughness's in the form of rib e.g. square, rectangular, triangular, wedge, chamfered; placed transverse to the flow direction or in an angle induces vortices to increases the local heat transfer coefficient along with friction factor [1]. Researchers are interested to maximise the heat transfer keeping the friction factor low. In obtaining the optimum heat transferring surface, grooves are also introduced along with rib turbulators. Researchers are also interested to apply the ribs in discrete forms to increase the turbulence intensity.

Liquid crystal thermography technique is applied to determine the circumferential variation of the Nusselt number over artificially roughened uniformly heated surface under forced convection [2]. In this paper an attempt has been made to comparatively study on element geometries used as artificial roughness by liquid crystal thermography. The objective of this paper is to provide details of the LCT technique used in the field of artificial roughness already studied by various researchers.

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Relaxation behaviour of Pristine and Cd1-xZnxS/ZnS Quantum Dots dispersed BBHA Nematogen Pankaj Kumar Tripathi¹, Bipin Joshi², and Shri Singh¹

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In this work, we have addressed the question –how the dispersion of Cd1-xZnxS/ZnS quantum dots (QDs) into the BBHA nematogen matrix will influence frequency and temperature dependences of dielectric permittivity and dielectric loss for the planar as well as homeotropic alignments. It has been shown that the QDs dispersed nematic LCs of negative dielectric anisotropy, such as BBHA, may prove to be advantageous in low charge consumable devices due to the easy charge transportation phenomenon and can be utilized in low power consumption LC displays.

Keywords: Quantum Dots, Dielectric permittivity, Dielectric loss, LC matrix.

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Design of stimuli responsive biocompatible liquid crystal droplets for the detection of proteins and DNA <u>Indu Verma¹</u>, Santanu Kumar Pal¹

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Designing stimuli responsive biocompatible surfaces for adsorption of proteins and DNA and detection of such interactions between protein and the modified surfaces are important for biomedical applications in tissue engineering, wound repair, drug delivery and many more. Currently, there are numerous physicochemical methods available to detect and study protein interactions such as surface plasmon resonance, quartz crystal micro balance, fourier-transform infrared spectroscopy and X-ray diffraction but the costly instrumentation and complexity limit their widespread use. Recently, liquid crystal (LC) droplets dispersed in aqueous solution have emerged as a simple optical probe for the detection of biological and chemical species at the LC-aq interface. Herein, we report a simple and useful advance in the design of LC droplets modified by a biocompatible polypeptide that enables a quantitative, label-free and real time detection of protein and DNA adsorption at LC-aq interface. Our approach involves surface driven ordering transitions in LC droplets which can be optically detected by following the director configuration of the LC molecules inside the droplets under polarizing optical microscope.

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Aroylhydrazone based columnar mesogens: A structureproperty relationship study Hemant Kumar Singh and Bachcha Singh

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Aroylhydrazone, hydrazine derivatives and their metal complexes are known to exhibit a broad spectrum of biological, bactericidal and fungicidal activities and have great interest due to their analytical, industrial and pharmacological importance. The aroylhydrazone based mesogenic ligands have been used to form novel family of metal containing liquid crystals with high thermal stability and high variety of liquid crystalline phases in contrast to many of the currently known metallomesogen. There are a number of reports (>500, source: Web of Science®) on these types of compounds and their metal complexes, but research on mesomorphic (liquid crystalline) behavior is still in its infancy except a few examples of such mesogens¹.

In this presentation, I will discuss about the structural features necessary for mesophase formation in aroylhydrazone derivatives in conjunction with POM, DSC and XRD studies to draw some conclusion on structure-mesophase relationship on the present highly mesophase potent core.

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Synthesis, Mesomorphism and Photoluminescence of a New Class of Anthracene-based Discotic Liquid Crystals Joydip De¹, Shilpa Setia¹ and Santanu Kumar Pal¹

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First example of anthracene-based discotic liquid crystals (DLCs) showing unconventional mesophases is reported. Among them, two of the derivatives showed stable columnar hexagonal plastic mesophases whereas other two exhibited a columnar nematic phase at room temperature as derived by X-ray scattering results. The central anthracene core is attractive in search for new functional DLC materials because of its unusual photoluminescence, electroluminescence and excellent electrochemical properties making them promising as an active component of organic light emitting diodes (OLEDs) as well as photovoltaics.

Four discotic liquid crystals (DLCs) based on anthracene, a novel redox active central core, have been synthesized and their mesomorphic behavior investigated. Among them, two of the derivatives showed stable hexagonal plastic mesophases whereas other two exhibited a columnar nematic phase at near room temperature as derived by X-ray scattering results. Type of the mesophases formed by these new class of compounds are rare that renders the central anthracene core attractive in the search for new functional DLC materials. HOMO-LUMO values have also been found to be much less in these materials which make them as good candidates for electron migration studies in self-organized systems. All the compounds show blue luminescence in solution under the long wavelength UV light. Overall, these new class of materials are promising, considering the emissive nature, ease of synthesis and stabilization of unconventional mesophases at room temperature or near room temperature.

Effect of Repulsive Interactions in the Hamiltonian Model of Biaxial Nematics: A Free-energy Study through Entropic Monte Carlo Sampling

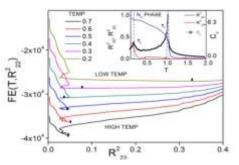
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The biaxial liquid crystal Hamiltonian model (\mathcal{H}) hosts, within quadratic approximation, inter-molecular interactions of varying strengths, between their uniaxial-uniaxial(μ), biaxialbiaxial (λ), and uniaxial-biaxial cross-coupling (γ) tensors, defining the model parameter space Σ for stability analysis. An extensively investigated trajectory is a parabola($\lambda = \gamma^2$, $\mu = -1$), incorporating the London dispersion approximation of molecular interactions. Mean-field theoretic (MFT) predictions and Boltzmann sampling-based Monte Carlo results concur on the resulting phase diagram along this path. From another interesting perspective, this trajectory also happens to be a curious boundary separating physical consequences on \mathcal{H} . Above the parabola, the values of (γ , λ) result in interaction terms which are all attractive promoting mutually compatible ordering of the three molecular axes. Below this path, the Hamiltonian does not unambiguously promote molecular ordering, in that the cross-coupling γ -term in \mathcal{H} turns repulsive while the other two remain attractive, for such order-promoting configurations. Bifurcation analysis of such a Hamiltonian is not without debate, and the MFT predictions are probably subject to corrections in this region [1]. In this context, we

report qualitative deviations from the earlier data, based on a more versatile Monte Carlo sampling procedure (entropic sampling). As this boundary is reached from the fully attractive region, subtle changes are observed in the thermal averages, particularly of the biaxial order (R_{22}^2) . Instead of a pure uniaxial intermediate phase (as predicted by MFT and supported by Boltzmann simulations), we find in this phase on cooling, an initial small increase followed by a



rather sudden decrease of R_{22}^2 , before the onset of a predicted low-temperature biaxial phase. Our analysis based on the free energy profiles plotted against R_{22}^2 in this intermediate phase (see Fig.), confirm the onset of a qualitatively different intermediate phase with a small biaxial order, consistent with earlier conclusions at the Landau point on the parabola [2].

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NCLC-2016, IIT(ISM) Dhanbad

Poster

P 1

Field-induced lasing properties of nematic- cholestric liquid crystal system doped with InP/ZnS semiconducting quantum dots <u>Aradhana Roy¹</u>, R. Dabrowski² and Rajiv Manohar¹

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Study of texture, response and dielectric properties has been carried out in the following nematic liquid crystal sample as well as cholesteric sample and its dopant with core shell quantum dot InP/ZnS. InP/ZnS has been reported as highly luminescent nanoparticles, hence an increase in optical birefringence is observed in quantum dot and cholesteric doped nematic sample with respect to pure. Polarizing optical micrographs (POMs) of planar aligned samples of nematic- cholestric liquid crystal system and doped mixtures taken at various temperatures under crossed polarizer condition are reported, which clearly show increase in luminescence from 64°C to 70°C. Enhancement of temporal response i.e switching time is observed in the mixtures of NLC doped with InP/ZnS nanoparticles. Variation in dielectric anisotropy is observed in a specific temperature range; however the conductivity of the dopant shows rapid change in comparison to pure. The UV absorbance of core shell nanoparticles doped nematic liquid crystal has increased with respect to pure nematic and also the emission wavelength has shifted for doped mixture. We have also studied quantum dots dispersed in a cholesteric photonic cavity for liquid crystal laser applications. For this the a linearly polarized beam is produced from circularly polarized light using a quarter wave plate, and then passed through a laser polarizer which is connected to digital oscilloscope that allows us to measure the intensities of polarization states. One of the strengths of using liquid crystal materials in a photonic device is their structural tunability and the photonic band gap of the cholesteric phase is tunable with temperature and applied electric field. Hence, the addition of QD's to chiral nematic liquid crystal increases the lasing capability of the sample. These properties of the chiral nematic LC and NLC-QD composites can be used in photonic devices and liquid crystal laser applications.

Keywords: core-shell quantum dots, nematic liquid crystal, laser, photonic band gap.

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Synthesis and characterization of chiral ionic liquid crystal with quaternary ammonium salts R.Mangaiyarkarasi and S.Umadevi

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Ionic liquid crystals (ILCs) form a versatile class of compounds combining the intriguing properties of ionic liquids such as ionic conductivity, high polarizability, low vapour pressure and the interesting features of liquid crystals namely organized structure, anisotropic chemical and physical properties¹. ILCs displaying a columnar hexagonal mesophase showing a very high ionic conductivity have been described.² Further, ILC exhibiting a cubic phase, which behaves as nano ion channel networks is reported.³ Recently, calamitic ILCs exhibiting SmA phase and their 2-dimensional assemblies forming ion conductive layers is presented.⁴ However, it is interesting to point out here that ILCs containing a chiral moiety in the molecular structure and exhibiting a chiral mesophase have not been reported so far. Chiral mesophases include interesting properties such as ferroelectric qualities, fast switching speeds, strong optical rotatory power etc. Combination of these chiral properties and ionic liquid behavior in a chiral ILC will open up a wide scope both in fundamental study and applications. In this regard, we have prepared new cholesterol containing chiral ILC compound having a terminal ammonium moiety. Herein, we present the synthesis, characterization and mesomorphic behavior of ILC compound. The differential scanning calorimetry (DSC) and polarizing optical microscopy (POM) studies indicated the presence of an enantiotropic chiral SmA phase.

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Enhancement of switching behaviour of Nematic Liquid Crystals Dispersed with Aluminium oxide Nanoparticles <u>Fanindra Pati Pandey</u>, Pankaj Kumar Tripathi and Shri Singh

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In the present study, the nanoparticles are dispersed into the liquid crystal for optimising the dielectric and electro-optical properties. The significant changes in the dielectric anisotropy and response time are explained on the basis of dipole–dipole interaction and anchoring phenomena. The aluminum oxide (Al2O3) nanoparticles have been used for dispersing in nematic liquid crystal, p-methoxy benzylidene p-butyl aniline (MBBA). The dielectric relaxation spectra which have been explained on the basis of interaction of nanoparticles with the liquid crystal molecules.

Keywords: Nematic Liquid Crystal; Relaxation Frequency; Nanoparticle; Activation Energy.

Design, Synthesis, Characterization and mesomorphic studies of dendrimer like, a series of Schiff's bases containing ether

and imine bond as a linking groups

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A new series of mesogenic aroylhydrazone based ligand crystals, N-[4-(alkoxy)benzylidene]-3,5-bis[4'-(alkoxy)benzyloxy)benzohydrazide, N[3,4bis(alkoxy)benzylidene]3', 5bis [4'(alkoxy)benzyloxy) benzohydrazide, N-[2,3,4-tris(alkoxy)benzylidene]-3',5-bis[4'-(alkoxy)benzyloxy)benzohydrazide and N-[3,4,5-tris(alkoxy)benzylidene]-3',5'-bis[4'-(alkoxy)benzyloxy)benzohydrazide, containing ether bond as a linker with same or different peripheral alkyl chains, and nickel(II) and copper(II) complexes of some of them have been synthesized. They were characterized by elemental analyses, Fourier transform infrared (FT-IR), ¹H and ¹³C nuclear magnetic resonance (NMR) and ultraviolet (UV)-visible spectroscopy. The mesomorphic properties of these compounds were investigated by differential scanning calorimetry and polarizing optical microscopy. All the aroylhydrazones except those with no alkoxy chains on either end of the molecule exhibit enantiotropic SmC mesophase and are sensitive to peripheral alkoxy chain length. The metal complexes are nonmesogenic and decompose upon heating at more than 300 °C. DFT calculations have been performed using GAUSSIAN-03 program at B3LYP level to obtain the stable electronic structure of the ligands and metals complexes. DFT studies accounts for the mesogenic nature of ligands and non-mesogenic nature of the complexes.

Enhancement of birefringence, dielectric anisotropy, UV absorbance and threshold voltage of nematic liquid crystal with the dispersion of fluorescent dye Govind Pathak¹, Atul Srivastava¹, Roman Dabrowski² and Rajiv Manohar¹

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In the present work fluorescent dye (Benzo 2,1,3 Thiadiazole) has been dispersed into the nematic liquid crystal (NLC) mixture 1550C which is consisted of 4'-(trans,trans-4alkylbicyclohexyl)carbonates and 4'-(4-(trans,trans-4-alkyl)-4-cyanobicyclohexane, different concentration. An increased value of birefringence has been found for dye dispersed system as compare to pure NLC 1550C. The incident light suffers an extra phase difference therefore; birefringence of the dye dispersed system has increased. The relative permittivity has been increased for lower concentration whereas its decreases for higher concentration of dye dispersed system in comparison to that of pure NLC. Dielectric anisotropy has been also measured in this investigation and found to be decreased for the dispersed system as compared to pure NLC. Splay elastic constant (K11) is measured and found to be decreased for dye dispersed system. Optical parameter has also been measured in the present work for pure and dye dispersed system and it was observed that UV absorbance has been increased for dye dispersed system than that of pure NLC. The value of threshold voltage has been also measured and found to increase on dispersion of dye in the pure matrix. The modified value of threshold voltage, birefringence and dielectric anisotropy are one of the promising results of this investigation. These high birefringent materials can be applicable in making of phase shifters and flat panel displays.

Keywords: Fluorescent dye, nematic liquid crystal, birefringence, dielectric anisotropy.

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Investigation of nano-sized diamond particles dispersed ferroelectric liquid crystal induced changes in relaxation behaviour and electro-optical parameters <u>Kaushlendra Agrahari¹</u>, Rajiv Manohar¹, Roman Dabrowski²

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Insulating nano-structured (d<10 nm) diamond particles (NSDP) were dispersed in ferroelectric liquid crystal (W343) and characterized by dielectric, electro-optical and optical techniques. Due to insulating nature, diamond nanoparticles reduce the unwanted ionic impurities associated to pure FLC material and thus fasten the electro-optical response of the composite. The presence of NSDP significantly affects the phase fluctuations of pure FLC material, therefore; the Goldstone mode characteristics have been changed according to the concentration of NSDP. In the present article, NSDP-FLC composites are investigated as a function of temperature, frequency, bias voltage etc and analysis has been done using Guest-Host theory. The practical applications of such composite have also been suggested in this study.

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Differentiation of analytes based on orientational transition of liquid crystals at LC/aqueous interface Mishra¹ Kirtika, Sachin Kumar Singh² and Bachcha Singh¹

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Recent studies show that competitive intermolecular interactions at liquid crystal (LC) interfaces can trigger ordering transitions to report biological and chemical events at surfaces. We developed a liquid crystal based system for the discrimination of structurally similar analytes at the LC/aqueous interface. Herein we have combined two principles and report that two structurally similar dyes behave differently on sodium dodecyl sulfate (SDS)-laden LC/aqueous interface in the absence and presence of β -cyclodextrins (β -CD). The competitive interaction of dyes at the SDS-laden 4-cyano-4'-pentylbiphenyl (5CB)/aqueous interface, in the absence of β -CD, can trigger a homeotropic-to-planar anchoring transition of the 5CB at the interface, which can be easily observed using a polarizing optical microscope. Further, depending upon the affinity of β -CD cavity to the two dyes over SDS, change in the optical appearance of 5CB was observed. This work demonstrates the differentiation of structurally similar dyes on the basis of differences in optical textural pattern of LCs.

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High concentration of colloidal gold nanoparticles dispersed with plastic columnar discotic liquid crystalline material <u>Mukesh Mishra¹</u>, Sandeep Kumar², and Ravindra Dhar¹

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In the present work, Colloidal gold nanoparticles (GNPs) have been dispersed in a plastic columnar discotic liquid crystal (DLC) namely 2, 3, 6, 7, 10, 11- hexabutyloxytryphenylene (HAT4). Thermodynamical, dielectrical and optical properties of nanocomposites confirm their insertion into the columnar matrix. The presence of GNPs in the triphenylene based DLC decreases the plastic columnar hexagonal to isotropic liquid phase transition temperature but the crystal to columnar hexagonal transition temperature does not change significantly. Interestingly the ionic conductivity measurements show an enhancement by about two orders of magnitude upon doping of GNPs. Dielectric permittivity measured parallel to the column axis in the homeotropic aligned sample has increased. Optical study suggests that band gap has decreased due to dispersion of GNPs.

Keywords: discotic liquid crystal-nanocomposites; homeotropic alignment; dielectric properties; band gap.

Enhancement in the thermal stability of the mesophases of 4-n-(nonyloxy) benzoic acid due to Li ion beam irradiation <u>Satendra Kumar</u>¹, Rohit Verma¹, R. Dhar² and Ambuj Tripathi³

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Energetic ion beam radiations produced in accelerators have been widely used for the modification of the materials [1, 2]. Sometimes the properties of the irradiated materials are improved and in other cases the materials are deteriorated [1-4]. Liquid crystalline materials have been widely used in every walk of life from calculators, computer monitors, dash boards of vehicle and space shuttles to wide screen television sets. The devices made up of liquid crystalline materials are sometimes used in high radiation prone environments such as nuclear installation centers and space applications. When these devices are used in such environments for a long time, different types and doses of irradiation highly affect these devices and often cause their malfunctioning. Therefore, it becomes important to study the effect of various types of radiations on various properties of these materials. In view of the above, a liquid crystalline compound 4-(n-nonyloxy) benzoic acid (NOBA) (As shown in Figure) has been irradiated at room temperature by Li ion beam (of fluences 10¹¹, 10¹² and 10¹³ ions-cm⁻²) in its crystalline phase using 3nA current by a pelletron beam. Thermodynamic, dielectric and UV-Visible spectroscopic characterization of the pure and irradiated materials has been carried out. Thermodynamic studies of the the pure and irradiated materials show that all the transition temperatures, enthalpies and entropies are increased due to the irradiation suggesting enhancement in the thermal stability of the mesophases. Dielectric results obtained on the irradiated vis-à-vis pure material suggest how the value of the transverse component of the dielectric permittivity of the irradiated material increases in the SmC phase whereas it decreases in the N phase. UV-Visible spectrum of the irradiated material shows an additional peak along with the peak of the pure material suggesting formation of new species in the irradiated materials.

Keywords: Li ion beam irradiation, Liquid Crystals, Dielectric and Thermodynamic Properties.

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Figure: Molecular structure of 4-(n-nonyloxy) benzoic acid (NOBA).

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Superior visco-elastic and ionic activities with reversal of elastic anisotropy observed in bent-core nematic liquid crystals doped with carbon nanotubes <u>Raj Kumar Khan¹</u>, Sharmistha Ghosh², Nandiraju V. S. Rao²

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Nematic phases in bent-core systems are rare because the molecules prefer packing into layers and often form smectic phases. In most bent-core nematic liquid crystals the bent elastic constant (K_3) is usually lower than splay elastic constant (K_1) owing to the presence of short range smectic -C like correlations in nematic phase [1-2]. Thus the elastic anisotropy (K_3-K_1) is usually negative in bent-core nematics unlike rod-like nematic liquid crystals where K_3 is always greater than K_1 . Here we report a short-core bent-shaped nematic liquid crystal whose negative elastic anisotropy was turned to positive by minute addition of single walled carbon nanotubes. We have systemically dispersed SWCNTs in a fluorinated four-ring bent-core nematic liquid crystal at different concentrations. Dielectric spectroscopy is employed to determine the dielectric permittivity and elastic constants of the system. We experimentally demonstrate that the SWCNT dispersed BCN system has improved viscoelastic properties. The dielectric anisotropy is significantly increased in 0.1% CNT dispersed system and the effect is attributed to enhanced nematic ordering due to π - π electron stacking between the SWCNTs and surrounding LC molecules. Threshold voltage also exhibits huge reduction in this system owing to the lower rotational viscosity caused by the ion trapping by CNTs. As a consequence the splay elastic constant is reduced in moderately doped system whereas bend elastic constant enhances remarkably in 0.1% nano/LC blend. This elementary study helps us to understand the interaction of SWCNTs with surrounding anisotropic medium composed of bend-shaped molecules and reveals significant modifications in viscoelastic, dielectric and ionic properties of the host.

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Existence of a line of critical points in a two-dimensional Lebwohl Lasher model

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Controversy regarding transitions in systems with global symmetry group O(3) has attracted the attention of researchers and the detailed nature of this transition is still not well understood. As an example of such system in this paper we have studied a two-dimensional Lebwohl Lasher model, using the Wolff cluster algorithm. Though we have not been able to reach any definitive conclusions regarding the order present in the system, from finite size scaling analysis, hyperscaling relations and the behavior of the correlation function we have obtained strong indications regarding the presence of quasi-long range order and the existence of a line of critical points in our system.

Liquid crystal functionalized polymer substrate <u>B. Sivaranjini¹</u>, V. Ganesh² and S.Umadevi¹

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Liquid Crystals (LCs) are self-assembled soft material with a huge potential for application in a wide variety of field such as sensing, biomedical, photonics, optoelectronics, electronic conductors, photovoltaics etc. apart from their significant use in display technology. [1,2] For majority of these LC applications, a pre-oriented well aligned sample of LC on a suitable substrate is highly crucial. The conventional methods existing so far for the alignment of LCs are effective in orienting the mesophase such as nematic, smectic only and are not efficient over a long period of time. Therefore, there is a significant need for formulating simple strategies for effective alignment of these materials on different substrates. An alignment layer made of molecules with a similar shape, i.e., LC molecules itself will provide necessary shape and symmetry compatibility for the bulk LC sample to be aligned. In view of this, we are forming the self-assembled monolayers (SAMs) of tailor-made LC molecules on various substrates and investigating the alignment abilities of these films to orient the bulk LC sample. Herein, we present the preparation of SAM of a rod-like thermotropic LC compound on a flexible, transparent polymer sheet (OHP) substrate and characterization of the modified substrate through IR, Contact Angle (CA) and Atomic Force Microscopy (AFM) studies. Further, our preliminary studies on versatility of these LC crystal modified substrates for the alignment of bulk LC sample are also presented.

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Tuning "de Vries-Like" Properties in Aroylhydrazone based

Liquid Crystal

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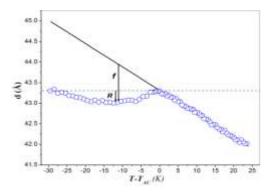
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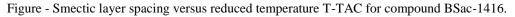
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Observation of de Vries-like properties in conventional aroylhydrazone based liquid crystal was achieved via incorporating differential interaction in different molecular end of strong SmC promoting aroylhydrazone core. On detailed investigations by polarized optical microscopy (POM), differential scanning calorimetry (DSC), and X-ray diffraction (XRD) studies, the de Vries-like properties thus obtained in the proposed system are found to be comparable to those of bonafide de Vries-like liquid crystals reported heretofore.

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Effect of silver nanoparticles on dielectric and electro-optical parameters of Room temperature nematic liquid crystal (6CHBT)

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Dielectric and electro-optical characterization of 4-(trans-4'-n-hexylcyclohexyl)isothiocyanatobenzene (6CHBT) and its composite with silver nanoparticles (diameter 100 nm) at the concentration 0.6 wt% have been studied. Dielectric parameters of pure nematic liquid crystal (NLC) and its nanocomposite in the homeotropic and planar aligned samples have been measured in the frequency range of 1– 35 MHz. It is observed that ionic conductivity increases in nematic (N) phase, whereas dielectric anisotropy decreases for nanocomposite. Relaxation frequency of an observed relaxation mode corresponding to molecular rotation about the short axis increases in the nematic phase of nanocomposite. From electro-optical studies it is observed that threshold voltage for switching the molecules from planar (bright) to homeotropic (dark) alignment decreases for nanocomposite.

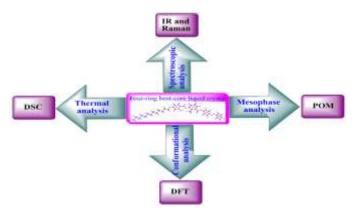
Keywords: nematic liquid crystal; dielectric anisotropy; relaxation frequency; threshold voltage.

Combined experimental and theoretical investigation of phase transitions in four-ring bent-core liquid crystal-Spectroscopic and DFT approach <u>Swapnil Singh¹</u>, Poonam Tandon¹, N.V.S. Rao², Jéssica Castro Fonseca³ and A.P. Avala³

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Four-ring bent-core liquid crystal (BCLC) has been synthesized and followed by thermal and mesomorphic investigations using differential scanning calorimetry (DSC) and polarised optical microscopy (POM) techniques, respectively. DSC along with POM revealed two phase transitions i.e. Cr ≥N ≥ Iso in the temperature range from 303 to 418 K in both heating and cooling cycles. Temperature dependent infrared and Raman spectroscopy are used to study the mechanism of phase transitions at molecular level and revealed marked changes in the spectral features especially the vibrations of OH, CH₂, CH₃, C=O, C=N groups in nematic phase in both heating/cooling cycles. Conformational and vibrational analyses have been performed using density functional theory (DFT), to identify the most stable conformer having hockey shape. Analysis of the potential energy surface (PES) for different torsion angles revealed the most probable conformational states for the BCLC. A good agreement between the calculated and observed infrared spectra validates the structure of this conformer that has been used for further studies. Spectroscopic investigations clubbed with DFT proved as a beneficial tool to understand the intermolecular interactions, H-bonding, molecular alignment, conformational changes as well the mechanism of phase transitions at molecular level.



A lipophilic dye Nile red as a probe to determine the phase state of lipid bilayer Animesh Halder¹, and Sanat Karmakar¹

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Nile red (9-diethylamino-5H-benzo[α] phenoxazine -5-one), a lipophilic dye is widely used for staining and monitoring organization, fluctuations, and heterogeneity in membranes. Fluorescence emission is fully quenched in polar aqueous environment. However, it fluoresces in the presence of lipid membranes.

We have studied the effect of emission spectrum, anisotropy and life time of Nile red on the composition and the phase state of the lipid membranes. We have also investigated the influence of cholesterol on the emission spectrum of Nile red in view of understanding the partitioning of cholesterol in liquid ordered and liquid disordered phase. Emission wavelength of Nile red in the presence of phospholipid membrane in fluid phase was found to be 630 nm. However, the emission maximum of Nile red in phospholipid membranes exhibits a significant blue shift in liquid ordered phase (composed of saturated phospholipids and cholesterol) as compared to liquid disordered phase containing unsaturated phospholipid and cholesterol. Our results have shown that the anisotropy (A) is lower in the liquid disordered (A = 0.146) phase than the liquid ordered phase (A = 0.213). The mean fluorescence lifetime of Nile red increases in the following order: gel phase < liquid disordered phase < liquid disordered phase.

Our studies indicate that the fluorescence properties of Nile red can be utilized to distinguish the membrane phase state and can also be used to monitor the amount of cholesterol in the liquid ordered phase of the membrane. We believe that our study will have great implications in detecting the phase state of liquid droplets in biological cells.

Fluid-solid transition in simple systems using density functional theory <u>Atul S. Bharadwaj¹</u> and Yashwant Singh¹

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A free energy functional for a crystal proposed by Singh and Singh (Euro physics Letters 88,16005 (2009)) which contains both the symmetry-conserved and symmetry-broken parts of the direct pair correlation function has been used to investigate the fluid-solid transition in systems interacting via purely repulsive WCA Lennard - Jones (RLJ) potential and the full Lennard - Jones(LJ) potential. The results found for freezing parameters for the fluid - face centred cubic (fcc) crystal transition are in very good agreement with simulation results. It is shown that although the contribution made by the symmetry broken part to the grand thermodynamic potential at the freezing point is small compared to that of the symmetry conserving part, its role is crucial in stabilizing the crystalline structure and on values of freezing parameters. The effect of attractive part of the LJ potential on the freezing parameters is found to be small, confirming the view that the fluid - solid transition is primarily determined by the repulsive part of the potential.

The Dielectric and Electro optical Parameters with High Figure-of-merit in Cd_{1-X} Zn_XS/ZnS Core /Shell Quantum dot Dispersed Nematic Liquid Crystal Ayushi Rastogi , Roman Dabrowski and Rajiy Manohar

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The present study is devoted to characterize the dielectric and electro optical parameters of the NLC-CSQDs composite system with dielectric properties being considered in both planar and homeotropic standpoint. Addition of Core/Shell structured quantum dot (CSQDs) results the change in UV-visible absorbance, Transmission, and switching time of pure NLC 2020 considerably. Present investigation shows the enhancement in the performance of nematic liquid crystal 2020 by doping small (0.1%) concentrations of (CSQDs). Faster electro-optic response along with high figure-of-merit (FOM) and birefringence are the promising results of this investigation. The figure-of-merit takes into account the change of phase retardation (Birefringence) and switching time of liquid crystal. It determines the optimal mix of polar and weak polar components in the liquid crystal. FOM is commonly used to compare the performance of a liquid crystal compound or mixture because it is independent of cell gap. Parameters like response time, viscosity, viscoelastic coefficient and splay elastic constant has been changed substantially for different composite system (0.1% and 0.25wt% conc.).The present investigation reveals the fact that FOM measures the efficiency of a device which in turn means a higher efficiency device will be more advantageous for application point of view.

Keywords: Figure- of -merit; Birefringence; Splay elastic constant; Response time; Nematic liquid crystal; Core /Shell quantum dot.

Critical Behavior in the Vicinity of Nematic-Smectic A Phase Transition of two polar-polar binary systems from Optical Birefringence Measurements <u>Barnali Barman</u> and Malay Kumar Das

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In the field of soft condensed matter physics the Nematic-Smectic A (N-SmA) phase transition has gained considerable attention due to several attractive features. Over the last few decades, the characteristic behavior of the N-SmA phase transition has been a subject of extensive theoretical and experimental studies in an effort to determine the order of the transition and the universality class to which it belongs. In this work a high resolution temperature scanning technique¹ of optical birefringence (Δn) measurement of two polarpolar binary systems (I) 4-n-heptyloxy-4'cyanobiphenyl (7OCB) and 4-n-octyloxy-4'cyanobiphenyl (80CB) (II) 4-n-octyloxy-4'-cyanobiphenyl (80CB) and 4-n-nonyloxy-4'cyanobiphenyl (90CB) have been reported. The birefringence (Δn) data have been used to explore the differential quotient Q(T) which is similar to specific heat capacity quotient C(T)and satisfy the same power-law behavior as of C(T). To describe the limiting behavior of the quotient Q(T) in the vicinity of N-SmA phase transition, critical exponent (α ') have been extracted which gives the information about the order of the N-SmA phase transition. Among these two investigated systems with decreasing the mol fraction of 80CB the α' value decreases along with decrease in the McMillan ratio (T_{NA}/T_{IN}) (where T_{NA} and T_{IN} are the N-SmA and Isotropic to N phase transition temperatures respectively) due to the decrease in the coupling strength between the N and SmA order parameter and α' value increases along with increase in the McMillan ratio due to the increase in the coupling strength between the N and SmA order parameter for the systems (I) and (II) respectively. It has been observed that the extracted a' values lies within the range between 3D-XY and tricritical point (TCP) indicates the 2nd order nature of the N-SmA phase transitions for all the investigated mixtures under study. A comparison with the effective critical exponent (α) related to specific heat capacity (C_p) obtained from adiabatic scanning calorimetry taken from ref. [2, 3] has also been made to verify our critical exponent value (α ').

Keywords: optical birefringence, critical exponent.

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Dielectric and electro-optical parameters of nematic liquid crystals with carbon nanotubes

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We have been described experimental studied on composites of nematic liquid crystals (NLCs) with Carbon Nanotubes (CNTs). The effect of CNTs on NLCs has been studied. Electro-optical & Dielectric parameters like: threshold voltage, dielectric anisotropy, and splay elastic constant have been investigated. Switching threshold voltage and splay elastic constant have been altered for NLCs- CNTs composites. The dielectric and electro-optic properties of NLCs- CNTs composites have been discussed with the help of expected models.

Molecular Organization of bent core hockey stick shaped molecules in pseudo-polar tilted smectic phases Deepshika Malkar, Arun Roy

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Understanding the properties of the variety of liquid crystalline (LC) phases exhibited by bent-core (BC) banana shaped molecules is an active field of research in soft matter physics. A typical BC molecule consists of a relatively rigid bent core part which has two rod-like arms joined end to end with an angle of about 120 degree between them. In addition, flexible aliphatic chains are usually attached to one or both ends of the rigid core of the molecule. In a symmetric BC banana shaped molecule, both the arms and the chains are the same, giving rise to the C_{2v} point symmetry of the molecules. A bent-core hockey sticks (BCHS) shaped molecule is formed when one of the arms is relatively shorter than the other arm of the BC molecule. The BCHS molecule can be considered to have a structure intermediate between the structures of the BC banana shaped molecule and the structure of the rod-like molecule.

In the present work, we report results of the experimental studies on a homologue series of azo substituted BCHS molecules with two asymmetric alkyl chains on the either side (See fig). The compound with alkyl chain length n = 9 (A9) exhibits two new tilted smectic phases in addition to SmA Phase. Whereas the higher homologue with alkyl chain n=14 (A14) shows two new pseudo-polar tilted smectic phases denoted as SmC_AM_A and SmC_IM_I between isotropic liquid and crystal phase. The new phases exhibited by these compound has been investigated by DSC, X-Ray diffraction, Switching Studies, Electric-field effect and polarizing optical microscopy studies. Both of the compounds show electro optic response under the application of an electric field.

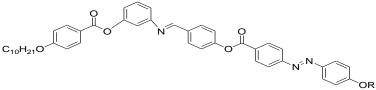


Fig: Molecular structure of homologue series of azo substituted BCHS molecule where $R=C_nH_{2n+1}$, n=9 & 14.

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Design of liquid crystal based interface to study the interaction of Gram negative bacterial endotoxin with milk protein lactoferrin <u>Dibyendu Das</u>¹ and Santanu Kumar Pal¹

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Milk protein lactoferrin (Lf) exhibits potent antibacterial activity due to its interaction with Gram negative bacterial cell membrane component, lipopolysaccharide (LPS). This paper represents fabrication of new Liquid crystals (LCs) based biosensonsor to explore the interaction between Lf and LPS. LPS self-assembled at aqueous/LCs interface and orients interfacial nematic 4-cyano-4'- pentylbiphenyl (5CB) LCs in a homeotropic fashion (exhibiting dark optical image under polarized optical microscope). Interestingly, on the exposure of Lf on LPS decorated aqueous/LCs interface, optical image of LCs changed from dark to bright indicating an ordering alteration of interfacial LCs from homeotropic to tilted/planar state. The ordering transition reflects strong binding between Lf and interfacial LPS that, in turn, perturbs the orientation of LCs. With help of epifluorescence microscopy, we further affirmed the interfacial LPS-Lf binding event by imaging the presence of FITC tagged Lf at the LPS laden aqueous/LCs interface. Followed by, in our next experiments, we also revealed that interfacial LPS-Lf binding phenomenon is highly specific over other membrane lipids as well as other milk proteins. In addition to that, we have quantitatively correlated the anchoring transition of 5CB during this interfacial binding event by measuring tilt angle of LCs. Finally, we have investigated the conformational behavior of Lf in solution as well as in presence of LPS using Ciruclar Dichroism (CD) spectroscopy and further reconfirmed with Vibrational Circular Dichroism (VCD) spectroscopy where we found that Lf undergoes alpha helix to random coil like structure in presence of LPS. As a whole the entire results described in this paper establish a robust approach to envisage the interaction between LPS and Lf through the ordering transitions of LCs at aqueous/LCs interface.

Dielectric and electro-optical study of magnetic nanoparticle doped weakly polar nematic liquid crystal <u>Geeta Yadav</u>, Rajiv Manohar

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This paper deals with the study of the effect of magnetic nanoparticles on the weakly polar nematic liquid crystal. Different parameters of dielectric data were measured for both homeotropic and planar aligned sample as a function of frequency and temperature and the substantial change has been noticed for the doped system. The nanoparticle affects the dielectric loss, permittivity, conductivity and tan delta in the positive way for lower concentration and decreases at higher concentration. Decrease in parameters may be due to aggregation at higher concentration. A minute change in dielectric anisotropy has also been observed. Nanoparticle also influences response time and birefringence properties of host liquid crystal. This change in properties has been explained on the basis of molecular disturbance created by magnetic nanoparticle and LC interaction.

Keywords: magnetic nanoparticle, permittivity, tan delta, birefringence.

Detection of bacterial functional amyloids using liquid crystals

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Functional bacterial amyloids represent a class of extracellular proteinaceous structures, diverse in structure and function. These structures being highly insoluble in water and resistant to denaturants, act as cytotoxins. They can also have multifaceted functions which include fimbriae formation, host cell adhesion and biofilm formation. A liquid crystal biosensing model for the detection of bacterial functional amyloids is presented which uses the membrane phospholipids as a template for the sensing event. This translational research approach is based on the amplification of small changes in the surface anchoring at the aqueous LC interface due to the interaction of the phospholipid and the biomolecule, thereby allowing its optical detection by the Polarizing Optical Microscope. Distinct optical patterns were observed which can be attributed to the structural transition of amyloids. This can be leveraged in clinical diagnostic tools because of the fact that these functional bacterial amyloids constitute a substantial fraction of the biofilms both in nature and engineered systems.

Phase morphology and optical behaviour of chiral nematic Liquid crystal mixture Jessy P. J, Radha S, Nainesh Patel

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Chiral Nematic liquid crystals are gaining much scientific attention due to their high promising features as photonic materials in optical sensors. We have investigated the phase behaviour and optical properties of a binary mixture of nematic and chiral liquid crystal in various ratios. The investigations were performed using Polarizing Optical Microscopy (POM), Differential Scanning Calorimetry (DSC), fluorescence spectroscopy and Refractive Index studies (RI). The mesophase transitions and optical textures at various temperatures have been detected by POM. The mixtures created new phases and extended the temperature range of phases. The grandjean steps and cholesteric polygonal appearance observed in mixtures are presumably due to the reorientation of the liquid crystal molecules. The phase transition temperatures by POM are confirmed by DSC. The temperature dependent RI analysis for various wavelengths in the visible spectral region reveals remarkable periodic alternation of the refractive index in mixtures. The photoluminescence of the binary mixtures enhanced with increasing concentration of chiral component. The observed sensitivity of optical response is expected to pave way for applications in optical sensors.

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Liquid crystal based microresonators Junaid Ahmad Sofi¹ and Dr Surajit Dhara¹

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We prepared various types of liquid crystal droplets in different polymer media. We measured the size variation of the droplets with time using optical polarizing microscope. We found two different rates of size decrement beyond a critical droplet size. Further, we studied dye doped ferronematic droplets (prepared by dispersing magnetic nanoparticles) of E-7 liquid crystal embedded in Lecithin added Glycerol polymer matrix. The lightly Nile Red dye doped ferronematic liquid crystal droplets typically of the order of few microns to few hundreds were excited with a suitable laser light¹. We analysed whispering gallery modes (WGM) and lasing in such droplets². We noticed significant changes occurring to the WGMs of the droplets upon small external magnetic field application typically of the order 10-100mT in Horizontal and Vertical ways respectively. In fact, the droplets with size greater than diameter 20 μ m displayed shifts in WGMs during increasing or decreasing fields.

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Study of Molecular Dynamics of Dark Conglomerate Phase Liquid Crystal

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Spontaneous chiral symmetry breaking in soft matter has attracted much attention. Chiral conglomerates with opposite handedness i.e. dark conglomerates (DC) have been observed in many bent shaped chiral or achiral molecules' liquid crystalline phase and also in isotropic phase. The DC phases have no birefringence or very low birefringence. In the DC phases layers are strongly deformed and organized in a sponge like structure. Due to the special organization of the layers, the mesophases appear optically isotropic between crossed polarizer on cooling from the isotropic liquid. Dark and bright domains can be observed by the rotation of the polarizer by a small angle and the brightness of these chiral domains exchange on rotation of the polarizer in the opposite direction. The optical activity in the DC phase of achiral bent core mesogens is attributed to the layers chirality or to the coupling of molecular conformational chirality to the layer chirality. It is an attractive issue to explore a novel DC phase exhibiting spontaneous generation in chiral asymmetry and the spontaneous formation of homochirality. We have investigated phase transition behavior and temperature dependent dielectric properties for the an achiral trimer [1].We have also noticed a dielectric relaxation process in DC phase as shown Fig.1

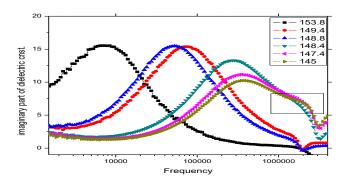


Fig.1 Plot of frequency vs imaginary part of dielectric constant.

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Laser assisted self-assembly, interaction and multi-axis electro-orientation of birefringent micro-sheets in nematic liquid crystals M. V. Rasna and Surajit Dhara

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Colloidal self-assembly has been one of the major driving themes in material science to obtain functional and advanced optical materials with complex architecture. Most of the nematic colloids reported so far are based on the optically isotropic spherical micro-particles. We study organic single crystal micro-sheets and investigate their orientation, interaction and directed assembly and multi-axis electro-orientation in nematic liquid crystals. The microsheets induce planar surface anchoring of the liquid crystal. The elasticity mediated pair interaction of micro-sheets shows quadrupolar characteristics. The average orientation angle of the micro-sheets in a planar cell and the angle between two micro-sheets in a homeotropic cell are supported by the Landau-de Gennes Q-tensor modelling. We demonstrated laser assisted 2D self-assembly exploiting the long-range elastic interaction. Our experiment opens up the possibility for making larger organic 2D crystals using micro-sheets as building blocks which have the potential for application of colloids in photonics. Tunability of such materials can be envisaged by external applied electric or magnetic fields and there is a growing interests in studying the collective dynamics of the colloids what is called a soft active metamatter (SAMM) driven by fields. This is an emerging class of engineered materials and requires proper understanding on electrokinetics of colloidal particles. We study electric field driven multi-axis electro-rotation of organic single crystal micro-sheets in the isotropic and nematic phase of a liquid crystal. We have shown that by applying a unidirectional electric field, birefringent micro-sheets can be rotated about multiple axes both in the isotropic and nematic phase of a liquid crystal. In the isotropic phase two rotations are observed due to the dielectric torque. For a fixed direction of applied field, the micro-sheets show six rotations around different axis in planar as well as in homeotropic nematic cells due to both the dielectric torque of the particle and elastic torque of the liquid crystal medium. These rotations are observed at varying voltage and wide time scales. The rate of rotation depends on the amplitude of the applied field and the viscosity of the medium. The control of orientation of optically anisotropic colloids by transducing external energy may be useful in novel electro-optics, photonics and their collective response may be potential for soft active metamatter.

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Structural Characterization of Citrate capped Gold nanoparticles dispersed in Liquid Crystals <u>M.Tejaswi¹</u>, P.Jayaprada¹, K. Sivaram¹, J. Sivasri¹, M.C. Rao² and RKNR Manepalli¹

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Liquid crystals act as tunable solvents for the dispersion of nanomaterials and they are being anisotropic media, provide a very good support for the self-assembly of nanomaterials in to large organized structures in multiple dimensions. Nanoobjects that are dispersed in the liquid crystals can trap ions, which decrease the ion concentration and electrical conductivity and improve the electro-optical response of the host. The synthesis and characterization are carried on liquid crystalline p-decyloxy benzoic acid p-undecyloxy benzoic acid (100BA & 110BA) with 30 μ l citrate capped Gold (Au) nanoparticles dispersion. Spectroscopic techniques like XRD, SEM, FTIR and DSC. These results showed that the dispersion of citrate capped Au nanoparticles in 100BA and 110BA exhibits nematic phases as same as the pure Liquid crystals, with reduced clearing temperature as expected. The smectic-C thermal ranges are enhanced and the nematic thermal ranges are changed slightly in DSC with the dispersion of 30 μ l citrate capped Au nanoparticles. Image processing technique of power law transformation is also used in this work to enhance the image quality and to identify the compound phases with better visibility.

Keywords: Synthesis; Polarizing Optical Microscope (POM); Differential Scanning Calorimeter (DSC); Nano dispersion; X-ray Diffraction spectrometric studies (XRD); Scanning Electron Microscopy studies (SEM) and Fourier Transform Infra-Red Spectroscopy (FTIR).

Electrical behaviour of Polymer Dispersed Liquid Crystals <u>Mithlesh Tiwari¹</u>, Satyentra Pratap Singh² and Kamal Kumar Pandey³

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Polymer dispersed liquid crystals are composites materials consisting of inclusion of liquid crystalline materials in a polymer binder. In this paper, we discuss the dielectric and electrooptical parameters of PDLC in nematic phase with variation of frequency, temperature and electric field. The polymer network provides an anchor point for alignment of the liquid crystalline bulk. The macroscopic extent of order in such systems depends on the order parameter of the liquid crystal (given by the temperature) and the polymer domain order parameter, induced by external stimuli, such as alignments or applied electric field. We studied thick PDLCs where substrate interactions cannot be employed and used electric fields instead. We show how the polymerization conditions, i.e., the temperature and the electric field, influence the overall order parameter in nematic based PDLCs.

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Design of Covalent Organic Framework (COF) and its Applications

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Presently there is an urge in the chemical science field to find the organic analogues of different materials in opto-electronics, solar cells, catalysis, porous materials etc. As a result there is an emerging field of a new class of materials called Covalent Organic Frameworks (COF), which is an organic analogue of porous inorganic materials known as Metal Organic Frameworks (MOF). Since the first discovery of COF materials in 2005 by Yaghi and co-workers¹, it has gained wide attraction due to its features such as the significant stability due to Covalent bonding, great structural diversity due to the versatile covalent-combination of building units, large surface area, tunable pore size, easy to tailor etc. Their potential applications range from gas storage to optoelectronics. Herein we are focusing on the synthesis of a COF which can coordinatively bind to metal centers with the help of the imine linkages (Schiff base) present in them; hence they can perform variety of applications like catalysis, sensing etc.

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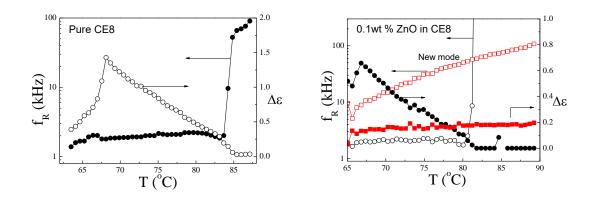
Effect of dispersion of ZnO on the dielectric property of ferroelectric liquid crystal

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We report the dielectric and polarization measurement of a LC-nano composites consisting of a commercially available ferroelectric liquid crystal doped with ZnO nanoparticles. It has been observed that the (i) temperature decreases and (ii) a new relaxation mode have been induced and iii) there is decrease in the ε_{\Box} values compare to that of pure. The relaxation frequency of the new mode observed in the planar geometry is matching with that of homeotropic, indicating that it is due to the relaxation about the short axis. It has been speculated that the complete 3-D misorientation of a few LC molecules in the vicinity of the nanoparticle reflected in the polarization and dielectric results.



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Silver Nanoparticles Dispersed Nematic Liquid Crystal for the Enhanced Birefringence and Lower Threshold Voltage Application

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Liquid crystals are usually looked upon as a potential material for display application and also for devices based on refractive and diffractive optics. Birefringence of the material plays the most important role in such applications. In the present study, Nematic Liquid Crystal (NLC) 4'-(Octyloxy)-4-biphenylcarbonitrile dispersed with different concentration of Silver Nanoparticles (Ag NPs) are characterised by electro-optical and dielectric spectroscopy method. The observed result shows that birefringence increases as we increase the concentration of Ag NPs in host NLC. This enhancement in birefringence for Ag NPs/NLC composite leads to the change in other physical parameter, like Relative Permittivity, Threshold voltage, and the Order Parameter. The dispersion of Ag NPs significantly reduces the threshold voltage which indicates its direct devices application. Additionally, the increase in AC conductivity value for Ag NPs/NLC composite discloses its importance in photovoltaic solar cell. The increase in conductivity for the composite can be attributed to the Ag NPs assisted induced charge transfer mechanism in the system.

Keywords: Nematic Liquid Crystal, Nanoparticles, Birefringence, AC conductivity, Relative Permittivity.

Study of PEMA Polymer Doped Cholesteric Liquid Crystal <u>Sumit Kumar</u>, Atul Srivastava and Rajiv Manohar

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We report thermal, dielectric and polarizing optical microscopic studies of poly ethyl methacrylate (PEMA) doped cholesteric liquid crystal (CLC). Cholesteryl pelargonate (CP) has been used as the host material. Investigations are performed for pure CP and 0.05 wt.% polymer doped CP. SmA - Ch and Ch - Iso phase transition temperatures are decreased. These results are also confirmed by polarizing optical microscopic (POM) study. It is very interesting to observe that such small concentration of polymer enhanced the stability of SmA phase on room temperature in cooling cycle on comparing to pure CP in which SmA phase was stable for few hours only. A very small change in the dielectric parameters of 0.05% PEMA doped CP is observed. This work can be helpful in understanding the effect of polymer on phase transitional behavior of liquid crystal.

Pattern Formation in Drying Droplets of CTAB Micellar Nanofluid

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Drying droplets have become very important for the production of various evaporation induced nanostructures. Cetyltrimethylammonium bromide (CTAB) is known to play a vital role for building nanostructures using evaporation driven self-assembly of nanomaterials formed in CTAB matrix [1]. We monitor the pattern formation from the drying droplet formed by CTAB-water system (Fig (a)). CTAB in water form a variety of liquid crystalline phases starting from spherical micelles at low concentration to a lamellar phase at high concentration [2]. The structure of these liquid crystalline phases can be tuned by the addition of salts, such as NaBr. Characteristics of liquid crystalline phases can easily be inferred using a polarizing optical microscope (POM). In this work we prepare an aqueous solution of CTAB in the presence of NaBr salt. Pattern formation in drying droplets on CTAB solution deposited on a glass substrate is studied using polarizing microscopy. When water evaporates from the droplets, ring like pattern appears as seen in Fig. (b) And at the final stage of drying dendritic aggregates are observed. We analyze the POM images obtained from the drying droplet using a Jones Matrix calculation. Interestingly, simulated image matches very well with that obtained from POM.

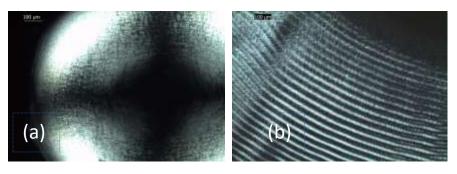


Fig (a) Drying droplet of CTAB+ Water

(b) Drying droplet of CTAB+Water+NaBr

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The effect of plasmonic nanoparticles on dielectric and optical properties of nematic liquid crystals <u>Deepa Singh¹</u>, U. B. Singh¹, M. B. Pandey² and R. Dhar¹

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We have been reported experimental studied on composites of nematic liquid crystals (NLCs) and Plasmonic Nanoparticles (PNPs). The effect of PNPs on NLCs has been investigated. Thermodynamical studies suggest decrease of clearing temperature of the composite material as compared to the pure material. Threshold voltage, dielectric anisotropy, and splay elastic constant have been studied. The dielectric and electro-optic properties of LC- PNPs composites have been discussed with the help of predictable models of LC- PNPs.

Keywords: Plasmonic Nanoparticles, display parameters, electro-optical properties.

Effect of quantum dots on the electrical and electro-optical parameters of nematic liquid crystalline material <u>U. B. Singh¹</u>, Deepa Singh¹, M. B. Pandey², S. Kumar³ and R. Dhar¹

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The effect of Cadmium Selenide Quantum Dots (CdSe-QDs) with Nematic Liquid Crystalline (NLCs) material on various electrical parameters of the pure and composite systems namely relative permittivity, dielectric anisotropy, dielectric loss and dielectric relaxation has been investigated. The electro-optical parameters namely threshold voltage, splay elastic constant and steepness of transmission-voltage curve has been studied for pure as well as dispersed systems. The nematic phase of liquid crystalline material supports alignment of CdSe-QDs parallel to the nematic director and improves local orientational ordering of host molecules in the nematic phase. Consequently, the electro-optical parameters of composite sample improved in the presence of the CdSe-QDs.

Keywords: Quantum Dots, Electrical Parameters, Transmission-Voltage Curve.

Dielectric anisotropy and relaxation time as function of temperature of a liquid crystal compound <u>Sangita patari¹</u> and Aparna Nath²

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Effect of temperature on the dielectric permittivities of liquid crystals compounds namely 4-Nonyloxybenzoic acid (90BA) have been studied by using a digital LCR bridge (HIOKI 3532-50 LCR HiTESTER) at the frequency 100 KHz. The temperature dependent physical properties such as dielectric anisotropy ($\Delta\epsilon$), splay elastic constant (K₁₁), relaxation time (τ) of the compound 90BA has also been studied extensively. It has been found that the compound 90BA exhibits positive dielectric anisotropy in nematic phase and negative dielectric anisotropy in smectic C phase. Similar behavior of dielectric anisotropy as function of temperature for 90BA was reported by other authors [1-3]. In the smectic phase there is a possibility of increase in transverse component of dipole moment (μ) and decrease in longitudinal component of dipole moment (μ_{\parallel}), hence the compound exhibits negative dielectric anisotropy. But further increase in temperature the orientation of the molecules changes which leads to increase μ_{\parallel} than the component μ_{\perp} for this reason the compound has found to exhibit positive dielectric anisotropy in nematic phase. The parameter K₁₁ exhibits similar behavior with temperature as that of $\Delta\epsilon$. The values of τ are found to decrease with decreasing temperature.

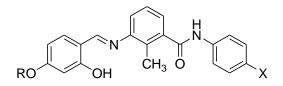
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New class of three-ring-based bent-core liquid crystals <u>Supreet Kaur</u>¹ and Santanu Kumar Pal²

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The discovery by H. Takezoe et al. (1996) revealed that bent-shaped molecules are not only forming the LC self-assembly but are also promising candidates to obtain spontaneous polarity as well as macroscopic chirality in achiral molecules. BLCs show some unique physical properties of such as ferroelectricty, molecular biaxiality, etc. which are not observed in calamitics. Considering the scarcity of bent-core materials exhibiting a room temperature nematic mesophase, this new class of materials has been proposed: a symmetrical bent-core molecule that incorporates three phenyl rings linked by an imine and amide moiety with alkoxy and polar end chains (fluoro and chloro groups). Molecular characterization and mesomorphic characteristics have been studied.



X= Cl or F

Nematic Smectic – C (N-SmC) Transition in 60.09 and 60.010 LC Compounds Through birefringence - An Optical Study

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The synthesis, characterization and measurement of refractive indices in N-(4-hexyloxy benzylidene)-4-alkoxy anilines, 60.0m compounds with varying alkoxy chain length as m = 9, and 10 is presented in this manuscript. The refractive indices n_e and n_o were measured at wavelength 589 nm with a wedge-shaped glass cell using the modified spectrometer. The temperature accuracy is ± 0.1 ^OC. The orientational order parameter S is obtained employing Kuczynski et al method. The results were compared with the data available in the literature.

Keywords: orientatioal order parameter S, Liquid crystalline compounds, Kuczynski method, birefringence.

Synthesis, characterization and mesomorphic investigation of substituted aroylhydrazone based discotic liquid crystals <u>Privanka Kanth</u> and Bachcha Singh

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The present study deals with the synthesis of a new series of substituted aroylhydrazone based mesogens containing amide linkage. A major disadvantage of amide based mesogenic materials is the high melting temperature. In order to obtain low melting mesogenic materials, we have synthesized a number of mono-, di- and tri-substituted benzylidenehydrazine based mesogens (liquid crystals) which differ in one or more than one tunable factors. The compounds synthesized have been characterized by suitable spectroscopic techniques. The mesomorphic properties have been studied by differential scanning calorimetric analysis (DSC), polarizing optical microscopic (POM) and X-ray diffraction (XRD) studies. During systematic study on phase behaviour of these ligands, we obtained results that led to the conclusion that mesophase stability of aroylhydrazone based mesogens depends upon the number of side chain density around the central core, carbon chain length and linking group.

Synthesis, Mesomorphic and Photophysical behaviours of benzoxazole salicylaldimines and their copper (II) complexes <u>Ragini Dubey</u>, Karunakar M, Rajasekhar Yerrasani, Angad Kumar Singh and T. R. Rao

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The benzoxazole series of 5-(alkoxy)-2-(((4-(5-methylbenzoxazol-2-yl-)phenyl)imino)methyl)phenol, BO (n = 10, 12, 14) and their copper (II) complexes have been synthesized and characterized by various spectroscopic techniques together with elemental analysis were employed to elucidate the molecular structures. The thermotropic properties were investigated by a combination of POM observation, DSC analysis and X-ray diffraction experiments. The ligands exhibit wide range of enantiotropic smectic A (SmA) phases at ~233° C as confirmed by their typical fan shaped optical texture under polarizing microscope. The complexes were all found to exhibit a thermally stable enantiotropic SmA phase at 279°C. The photophysical study of ligands indicates that they exhibit broad absorption band at 350 nm and emission at 413 nm. DFT calculations have been performed using GAUSSIAN-03 program at B3LYP level to obtain the stable electronic structure of the ligand with dodecyloxy chain length and its copper (II) complex.

Synthesis, liquid crystalline behaviour and photo physical properties of benzimidazole- based Schiff-bases with various alkyl chains

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A series of luminescent benzimidazole-based Schiff-bases 5-(alkyloxy)-2-(((2-(4-(alkyloxy)phenyl)-1H-benzimidazol-5-yl)imino)methyl)phenol with different alkyl chains was synthesized and characterized by various spectroscopic techniques like ¹H & ¹³C NMR, UV-Vis, fluorescence and mass spectrometry. All the compounds exhibit smectic A (SmA) phase and their phase transition behaviour and thermal stability were investigated by differential scanning calorimetry (DSC), polarising optical microscopy (POM), powder X-ray diffraction (PXRD) studies and thermo gravimetric analysis (TGA). The fluorescence studies indicate that all the compounds show green emission. An electrochemical study of 3d by cyclic voltammetry shows a band gap of 2.56 eV with HOMO and LUMO energy levels of \Box 5.22 eV and \Box 2.67 eV, respectively.

Nanoparticles Coated With Dimer-Like Mesogenic Ligands: Synthesis and Characterization of Liquid Crystal-Nanoparticle (LC-NP) Composites Sachin Ashok Bhat and Channabasaveshwar V. Yelamaggad

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Liquid crystals (LCs) represent an exciting class of soft-matter, while remaining in a fluid state, possess intrinsic long-range order and thus, they exhibit a range of exceptional properties which are not only fascinating from basic research, but also hold huge potential for a wide variety of advanced technological applications. Nano particles (NPs), being ultrafine particles with diameter size less than 100 nm, show a range of remarkable optical, electronic, magnetic and chemical properties. In recent years, therefore, there have been constant efforts in developing an altogether different class of hybrid materials where the LC and NP concepts have been combined by realizing their hybrid motifs¹. It is shown that the assembly of NPs into highly processable, self-healing structures can be accomplished / tuned with the help of LCs as they possess intrinsic order and fluidity at the molecular and mesoscopic levels². Inspired by such innovative findings, we have designed and prepared liquid-crystalline nanoparticle (LC-NP) composites by coating NP (as a central scaffold) with a dimer-like mesogenic ligand (as a capping agent). The preliminary molecular structural elucidation of LC-NPs has been carried out with the aid of UV-Vis, IR, ¹H NMR, SEM image and EDX mapping. The liquid crystal behaviour of these LC-NPs has been evidenced with the help of optical polarizing microscope and differential scanning calorimeter. These optical and calorimetric results coupled with CD studies indicate the self-organization of LC-NPs in to a columnar fluid structure having chirality (handedness).

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Quantum Dots Dispersed Ferroelectric Liquid Crystal: study of improved photoluminescence Shivani Pandey¹ and Rajiv Manohar¹

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 $Cd_{1-x}Zn_xS/ZnS$ core/shell quantum dot (QD) has been dispersed in ferroelectric liquid crystal (FLC) into different concentrations. Optical and electro-optical measurements have been carried out on the pure and composite system. Enhancement in photoluminescence (PL) for the composite has been observed in the present investigation. This enhancement in the PL intensity has been attributed to the coupling of localized surface plasmon resonance from QDs with FLC molecules. A faster optical response has also been observed on addition of QDs into the FLC matrix. These results will certainly be helpful in utilizing QDs for obtaining faster response of the FLC material. These studies would also provide better understanding of improved photo luminescent liquid crystal display devices.

Keywords: Quantum dots, ferroelectric liquid crystal, photoluminescence.

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Nature of Smectic-A to Smectic-C Transition in a binary Liquid Crystal Mixture Consisting of Hockey Stick-Shaped and Rod-Like Molecules

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During past few decades a considerable attention has been made to understand the nature of the Smectic-A (Sm-A) to Smectic-C (Sm-C) phase transition. However, several experimental techniques have been made to make an exact conclusion whether this transition is second order or first order. Theoretically, the Sm-A and Sm-C phase transition belong to the threedimensional (3D) XY universality class. On the other hand, Huang et al.¹ have been observed deviations from the 3D-XY like behavior in close vicinity of that transition. Moreover, Liu et al.² shows Landau behavior including tricritical appearance in heat capacity measurement. The ultrasonic velocity and birefringence measurements have also been found to yield frequently non-Landau outcomes^{3,4}. Therefore, it is quite plausible to expect that the transition can exhibit a crossover from 3D-XY critical to tricritical behavior. Therefore the crucial factors responsible for driving this transition from a second order to first order are still not quite clear and necessitate further measurements appropriate for studying the pretransitional fluctuation at this transition.

In this work, we have studied a high resolution measurement of optical birefringence (Δn) in order to probe the critical behavior at the Sm-A–Sm-C phase transitions in a binary system comprising of the rod-like heptyloxy-cyanobiphenyl (7OCB) and a laterally methyl substituted hockey stick-shaped mesogen, 4-(3-n-decyloxy-2-methyl-phenyliminomethyl) phenyl 4-n-dodecyloxycinnamate (H-22.5) by varying the mol. fraction of 7OCB. We have extracted the critical exponent value by analyzing temperature derivative of Δn data. Remarkably, a crossover nature from second order to first order character of the Sm-A–Sm-C phase transition has been observed in this system. The results obtained reveal that the order of Sm-A–Sm-C phase transitions strongly depends upon the Sm-A range which is very similar to the nematic range dependence of the N-Sm-A phase transition. The tricritical value of critical exponent has also been verified by fitting the renormalization group expression taking higher order terms and keeping the tricritical critical exponent value ($\alpha'_{TCP} = 0.5$).

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Effect of Metal Ag Nanoparticles on the Alignment and Relaxation behaviour of Ferroelectric Liquid Crystalline material in SmC* phase

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The effect of dispersion of metallic silver nanoparticles (NPs) on the thermal and dielectric relaxations behaviour of FLC (W343) with the variation of dopant concentration has been examined in the present study. DSC traces confirms the large changes in first order transition temperatures (SmC* - SmA and SmA - N*) of FLC due to the presence of NPs. Changes in the alignment of FLC material in different phases has been visualized by the polarizing optical image analysis. Formation of nanoparticle induced line structures (NPLS) are one of the important finding of the present study. They have been found in the composites having high conc. of NPs. The dielectric spectroscopy technique has been used to see the relaxation behaviour of the samples. Non – appearance of characteristic goldstone mode in composite having higher conc. of NPs is very fascinating. Change in effective dipole moment and ion concentration in the composites has been observed in the temperature dependent analysis of relative permittivity, AC conductivity and dielectric loss factor. A significant change has been observed in optical tilt angle, spontaneous polarization and response time after the addition of NPs. The observed tilt angle has been discussed on the basis of plasmon – polariton effect.

Keywords: metal nanoparticle; nanoparticle assemblies; ferroelectric liquid crystal; ion adsorption.

Synthesis and characterization of novel chiral dimers exhibiting highly frustrated liquid crystal phases Uma S. Hiremath

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Since the discovery of chiral liquid crystalline state by Reinitzer in 1888,^{1,2} mesogens possessing molecular chirality have been intensively investigated.³⁻⁹ In particular, a variety of new chiral mesogenic materials have been realized based on the rational molecular engineering.⁴ This has, in fact, resulted in the invention of a great variety of novel LC superstructures¹⁰ that are enormously significant in the context of both basic research and various emerging technologies. We have designed and synthesized two novel series of optically active dimers comprising cholesterol and biphenyl-4-yl 4-(n-alkoxy)benzoate cores interlinked though either an odd-parity/even-parity spacer. They stabilize an extremely complex, frustrated liquid crystalline state viz., the twist grain boundary (TGB) phase with chiral smectic C structure, denoted as TGBC* phase, over a wide (50-110°C) temperature range. Notably, the dimers with an odd-parity spacer show an additional frustrated liquid crystal phase namely, the blue phase (BP). The presence of such frustrated phases suggests that the synthesized dimers are characterized by high enantiomeric excess and strong molecular chirality. These optically active, nonsymmetric dimers constitute new examples of rarely found strongly chiral, optically pure dimers showing frustrated liquid crystal phase over an adequately wide thermal range.

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A Comparative Study of Droplet Pattern and Electro-Optic Behaviour of Azo and Anthra dye doped Polymer Dispersed Liquid Crystal Films

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Polymer dispersed liquid crystal (PDLC) films using nematic liquid crystal (NLC) and photocurable polymer (NOA 65) were prepared by polymerisation induced phase separation (PIPS) technique, in equal ratio of polymer and liquid crystal (LC). We report a comparative analysis of droplet pattern and electro-optic (EO) behaviour of PDLC films with the addition of azo orange and anthraquinone blue dichroic dyes taking in different concentrations (wt/wt ratio) such as 0.0625%, 0.125%, 0.25%, 0.5% and 1% of the LC mixture. In OFF state, LC droplets in anthra dye doped PDLC exhibited bipolar pattern relatively at low concentration ($\leq 0.25\%$) of dye and radial in addition to axial droplets were observed at higher dye concentrations (0.5% and 1.0%). However, in case of azo dye doped PDLC, merely bipolar pattern of LC droplets was observed for each concentration of dye. In ON state, LC molecules align along the direction of applied electric field and all pattern of LC droplets shifted to vertical radial pattern in both dye doped PDLC films at saturating electric field. Experimental results showed the better transmission (~116 a. u.) and higher contrast (~1611) in anthra dye doped PDLC with consistent average droplet size ~ 4.30 μ m at operating electric field (4.27V/ μ m), with compared to azo dye doped PDLC transmission (~25.4 a. u.) and contrast (~1058) at relatively lower operating electric field $(3.13V/\mu m)$ with consistent average droplet size ~ 4.20 um. at 0.0625% dve concentration.

Keywords: Nematic liquid crystal, polymer dispersed liquid crystal, azo orange and anthra blue dichroic dye, droplet pattern, contrast ratio.

Three-ring based lower molecular weight Cholesteric liquid crystals: Synthesis and Characterisation <u>Vidhika Punjani¹</u> and Santanu Kumar Pal²

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Cholesteric LCs (CLCs) is of particular interest due to their unique ability to self-organize into a helical supramolecular architecture. CLCs are known to be highly sensitive to a number of external stimuli. Among various forms of stimuli such as heat, electric field, chemical reaction, or mechanical force, light is particularly fascinating owing to the advantages of ease of addressability, fast response time, and remote control in a wide range of ambient environments. CLCs have emerged as a novel class of smart materials which have found widespread applications in reflection displays and photonic applications. Here we have synthesized three ring based bent core cholesteric liquid crystal containing a rigid core and cholesterol linked via flexible alkyl spacers. The rigid core plays an important role in the mesomorphic properties of the molecule. The chemical structures of the compounds were characterized by ¹H NMR, ¹³C NMR, Ultraviolet Spectroscopy, Infrared Spectroscopy and Mass Spectroscopy (POM), Differential Scanning Calorimetry (DSC) and XRD studies.

Effect of temperature and electric field on 2D nematic colloidal crystals stabilised by vortex-like topological defects

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The foreign particles in nematic liquid crystals induce topological defects. Particle defect combinations are known as elastic dipoles or quadrupoles depending on the symmetry of the transverse components of the far-field director. These dipoles have a natural tendency to selfassemble due to anisotropic elastic forces. An unusual defect structure in which a non-singular disclination loop with a vortex-like defect is formed when two collinear anti-parallel elastic dipoles are pushed. This structure is named an escaped hyperbolic defect ring (EHDR) with a topological strength of -2. The loop encircles the line connecting two particles and forms dimers which are metastable in planar nematic (PN) cells. However, in twisted nematic (TN) cells, chirality escalates the spontaneous formation of non-singular colloidal dimers from antiparallel dipoles. We report experimental studies on 2D colloidal crystals of dimers stabilized by vortex-like defects in planar nematic and $\pi/2$ twisted nematic cells. The dimers are prepared and self-assembled using a laser tweezer. We study the effect of temperature and electric field on the lattice parameters of the colloidal crystals. The lattice parameters vary with the temperature in the nematic phase and a discontinuous structural change is observed at the nematic to smectic-A phase transition. In the nematic phase, we observed a large change in the lattice parameters $(\sim 30\%)$ by applying an external electric field perpendicular to the plane of the 2D crystals. The idea and the active control of the lattice parameters could be useful for designing tunable colloidal crystals.

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Two Dimensional Fringe Projection Technique for Three **Dimensional Object Shape Measurement**

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In this paper, we propose a new technique for three dimensional (3D) shape measurement using two dimensional (2D) fringe projection profilometry with high frequency fringes along y direction and low frequency fringes¹ along x direction. In this method, phase maps are extracted separately for horizontal and vertical fringes² and shape of 3D object is retrieved by combining individual shapes from the phases along x and y direction. Experimental and simulation results are presented to show the effectiveness of the proposed technique.

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Theoretical estimation of current transfer length of Cu/Ti/MgB₂ superconducting monofilamentary wires <u>Irshad Ahmad¹</u> and P.M. Sarun¹

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The estimation of current transfer length (CTL) for the combination of Cu:Ti:MgB₂ superconducting wire has studied theoretically using computational simulations. CTL is calculated by employing analytical and numerical models. In numerical model, finite difference method (FDM) is used for calculating CTL. With the help of FDM method, electric potential at each grid points were measured and subsequently used for the estimation of CTL. The results obtained from both analytical and numerical model were compared and they show good agreement. The result shows that a considerable part of the applied current is not transferred into the superconducting core for short length samples, instead, it flows through the sheath in Cu sheathed conductors. This technique is also applicable for other combination of sheath materials and is fruitful for screening the proper combinations of sheath and barrier or interface materials for fabrication of superconducting monofilamentary wires for current lead applications.

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Structural and Dielectric Properties of Sodium Niobate Ceramic

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Sodium Niobate (NN) was prepared by conventional solid state reaction method. The identification of the phase was done by X-ray diffraction (XRD) analysis. The microstructure of sintered sample was characterized by field emission scanning electron microscopy (FE-SEM). A detailed investigation of dielectric properties of the NN ceramic was studied in the wide range of temperature (40 °C – 500 °C) and frequency (100 Hz – 5 MHz). The highest value of dielectric permittivity ε_r was observed at the transition temperature Tc = 400 °C. The ac conductivity spectra shows a transition from frequency independent region dc-conductivity to dispersive region where conductivity start to increase with increasing frequency. The activation energy estimated within the moderate temperature is found to be very low (<<1 eV), indicates that the conduction process in the material is due to the mobility of singly ionized oxygen vacancies.

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Optical properties of Titanium-di-oxide (TiO₂) prepared by hydrothermal method

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Recent development in semiconductor nanoscience is able to control the shape and size of nanomaterials. Nanosized titanium-di-oxide (TiO₂) has unique physicochemical properties with applications in various fields such as electronic device fabrication, photo catalysis, photovoltaics, energy storage, gas sensing, Dye Sensitized Solar Cell etc^[1]. Till now numerous synthetic strategies liken sol–gel, hydrothermal, solvothermal, electrochemical anodization, electrodeposition etc. have been employed for the formation of TiO₂-based nanomaterials in the form of particles, tubes, fibers/wires, belts, rods, etc. Recently, research on titanate and its derived TiO₂ nanostructures with large specific surface area have received great attention. Investigation on the thermal or hydrothermal treatment of titanate nanomaterials is of paramount importance in designing ideal shape, size, exposed active facet, and phase of TiO₂ materials with enhanced photocatalytic activity^[2]. TiO₂ is a wide band gap n-type semiconductor with high chemical stability, low-costs, non-toxicity, strong photocatalytic activity and high photoelectric conversion efficiency. Its band gap is about 3.2 eV and occurs in three crystalline polymorphs — rutile, anatase and brukite. Anatase and rutile are most is also drawing attention in the above mentioned applications.

Here, in this communication TiO_2 has been commonly synthesized phases. Rutile is the most stable phase, but now a day anatase phase en prepared by hydrothermal method at 180°C. In this work we have shown the changes in optical properties with different external parameters. The morphological information of the prepared materials has been obtained from Field emission scanning electron microscopy (FESEM). The prepared samples have been characterized by UV-Vis spectrophotometer to know the band gap of the material in the range 200 - 800 nm. The vibrational bonds present in the material have been identified from the Fourier transform infrared (FTIR) spectroscopy. The photoluminescence (PL) spectra of the prepared samples are recorded at room temperature in the range of 400 - 700 nm. The main scope of this work is the use of this material in LED and low cost photocatalytic technology.

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Physical Properties of PAni-PMMA Blend as an Alternative Emissive Layer for PLED

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Polyaniline (PAni) is a conducting polymer that has captured intense attention of the scientific community in the recent years because of its potential applications in solar cells, sensors, diodes etc. Here oxidative polymerization method has been used to synthesize varying different monomer (aniline) and oxidant (Ammonium polvaniline by peroxydisulphate) ratio at room temperature. The main aim is to enhance the photoluminescence (PL) intensity of the polyaniline by forming PAni-PMMA blend. From UV absorption spectra of PAni Samples characteristic peaks appear at about 620 nm due to Benzoid-Quinoid ring charge transfer and at about 800 nm due to π - polaron transition. Morphological study by FESEM shows tube like structure of the pure PAni samples. The I-V curve indicates the semiconducting nature of PAni samples. From the different physical characterization, the PAni sample prepared with 4:5 monomers and oxidant ratio is found to be suitable for PLED application. But the PL spectra of PAni show the blue emission with low intensity. PMMA is an insulating polymer with high PL intensity. So to enhance the PL intensity of Polyaniline, PAni-PMMA blend is synthesized with different PAni and PMMA ratio. PL spectra of PAni-PMMA blend shows that with addition of PMMA the PL intensity of the blend becomes very large as compared to that of pure polyaniline samples and the blend also emits radiation in the blue region of visible spectra. From the I-V curve it is observed that with increase in PMMA content in the blend the conductivity decreases. The PAni-PMMA blend with ratio 1:1.25 is found to be most suitable for PLED application due to high enhancement of PL intensity compared to pure PAni Sample. So it can be concluded that the PAni-PMMA blend is a promising material for PLED application due to its high PL intensity and high conductivity.

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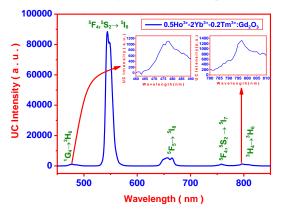
Upconversion emission properties in Ho³⁺-Yb³⁺ Tm³⁺: Gd₂O₃ phosphor

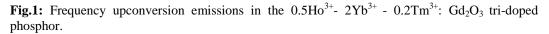
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In present study we performed frequency upconversion emissions in the Ho³⁺-Yb³⁺ Tm³⁺: Gd₂O₃ tri-doped phosphor materials prepared by solution combustion route. The multi-colour upconversion emission capability has been observed in the tri-doped phosphor under 980nm diode laser excitation. In co-doped phosphor, three upconversion emission bands around ~ 545 nm, ~ 667 nm and ~ 759 nm have been observed and assigned via $({}^{5}F_{4}, {}^{5}S_{2} \rightarrow {}^{5}I_{8})$, $({}^{5}F_{5} \rightarrow {}^{5}I_{8})$ and $({}^{5}F_{4}, {}^{5}S_{2} \rightarrow {}^{5}I_{7})$ transition of Ho³⁺ ion respectively. In the tri-doped phosphor five UC emission bands around ~ 477 nm, ~ 545 nm, ~ 667 nm, ~ 759 nm and ~ 797 nm corresponding to the (${}^{1}G_{4} \rightarrow {}^{3}H_{6}$), (${}^{5}F_{4}, {}^{5}S_{2} \rightarrow {}^{5}I_{8}$), (${}^{5}F_{5} \rightarrow {}^{5}I_{8}$), (${}^{5}F_{5} \rightarrow {}^{5}I_{8}$), (${}^{5}F_{4}, {}^{5}S_{2} \rightarrow {}^{5}I_{7}$) and (${}^{3}H_{4} \rightarrow {}^{3}H_{6}$) transition of Ho³⁺ and Tm³⁺ ions have been observed. The mechanism involved in the upconversion process has been explained through energy level diagram and energy transfer process [1-4]. The developed tri-doped phosphor can be used in making NIR to visible upconvertor and display devices.





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Study of Biophysical Parameters under Physiological Conditions

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Fluorescence correlation spectroscopy (FCS) is a fluorescence technique to determine the chemical, physical, and dynamic properties of bio-molecules and biological systems at the single molecule level [1]. FCS measures the fluctuations of the fluorescence intensity when particles move in and out of the detection volume and analyzes it to yield information about the motion of the molecules through the observation volume. Especially FCS has been used to measure parameters like diffusion coefficient and hydrodynamic radius of the bio-molecules. In the present study, we simulated FCS data for different microscope point spread functions (PSF), diffusion times and number of particles in the PSF. The corresponding biophysical parameters like diffusion coefficient and hydrodynamic radius of bio-molecules were estimated successfully. It has been observed that our deduced biophysical parameters are in the range of physiological conditions [2-4].

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Nonlinear Optical Image Encryption using Interferometry and Gyrator Transform

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In this paper, a new nonlinear technique for optical image encryption is proposed by combining the primary image with a secondary image. First, the primary image is multiplied with a random phase mask and the product is squared which results in a complex image. Similarly, the secondary image is also multiplied with another random phase mask to get the other complex image. These two complex images are then Fresnel propagated with distances d_1 and d_2 and then added to get a composite complex image, which is further gyrator transformed^{1,2} (GT) with angle α . After performing a phase truncation³ operation on the GT output, the amplitude part is transmitted and phase part is used as a decryption key. The proposed technique provides a large set of security keys and it is also robust against noise and occlusion attacks. The numerical simulation results are presented in support of the proposed technique.

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Estimation of Effective Pixel Size in Image Correlation Spectroscopy

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Image correlation spectroscopy (ICS) was developed as an imaging tool to obtain biophysical information [1]. Spatio-temporal correlations of fluctuating fluorescently labeled molecules disclose how they move, interact and bind in the different cellular sections. Each image in the series is a convolution of the microscope point spread function (2D-PSF) with the point-source emission from the fluorophores due to diffraction [2]. This convolution causes the signal from a point-emitter to be spread over a number of pixels. It was reported that the pixel size should be 3 to 4 times higher than the lateral resolution to over-sample the PSF and establish spatial correlations between intensities recorded in adjacent pixels [3]. This was the critical step in the ICS study. However, to the best of our knowledge, the most effective ratio between pixel size and size of lateral resolution was not reported. Therefore, in the present study, we simulated the image series by varying the ratio of lateral resolution and pixel size to estimate the effective critical step. We believe that our evaluated number has more accuracy than the previous reported range.

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Structural and Morphological properties of TiO₂ thin film synthesized by hydrothermal method Asish kumar Mohapatra and J. Navak

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Metal oxide semiconductors constitute a class of interesting materials for their high stability, low manufacturing cost and wide industrial applications. Titanium dioxide occurs in three crystalline polymorphs: rutile, brookite and anatase. Rutile is the most stable phase in bulk TiO_2 . During recent years, nanorods, nanoparticles and nanocrystals of titanium dioxide and zinc oxide have been studied and researched in priority basis because of their potential applications in Dye sensitized solar cells, Quantum dot sensitized solar cells, gas sensor and photocatalysis. Titanium dioxide is considered to be superior to zinc oxide because it shows higher light-to-electricity conversion efficiency in dye-sensitized solar cell. Recently nano structured of TiO_2 such as Nanorod, Nanotube, Nanosphere are used for device fabrication due to large surface area. Among all, the single crystalline rutile TiO_2 nano rod reveals better performance for carrier transpiration in DSSC solar cell. In this report, nanostructured TiO_2 has been synthesized in the form of nanocrystalline thin films by hydrothermal method. The thin films contain aligned nanorods with rectangular facets and having wide variety of morphology and structure. The structural and morphological properties were studied by X-ray diffraction, FE-SEM characterization technique.

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Synthesis, characterization and study of optical property of Graphene/CdS/PPY nanocomposite B. Purty¹ and R.B. Choudhary¹

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PPY/CdS/Graphene nanocomposite was synthesized by simple in-situ polymerization method with varying concentration of CdS nanoparticles. These nanocomposites were characterized by X-ray diffraction (XRD), Field emission scanning electron microscope (FESEM), Fourier transform infrared spectroscopy (FTIR), UV-vis absorption and I-V measurement techniques. The change in optical band gap with increasing concentration of CdS nanoparticles was studied by tauc plot. FESEM images show a good dispersion of the CdS nanoparticle and it is successfully combined with each other. The presence of CdS nanoparticle improves the optical property of the material. It also exhibits an excellent electrochemical behaviour which is defined by the cyclic voltamatery curve.

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Structural and Photometric Properties of Highly Luminescent Zn²⁺ Incorporated CaTiO₃:Eu³⁺ Perovskite Nanophosphors for Optoelectronic Applications <u>Dhananjay Kumar Singh</u> and Jairam Manam

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Luminescence properties of trivalent rare-earth ions doped in various titanates host matrix has been attracted more attention for researcher owing to their potential application in optoelectronic devices. The present work reports Zn^{2+} co-doped CaTiO₃:0.15Eu³⁺, a promising nanophosphor materials have been synthesized by solid state reaction method and characterized systematically by various technique such as XRD, FTIR, FESEM, Photoluminescence, PL decay time and UV-Vis spectroscopy to examine the structural, morphological and luminous performance of the samples. XRD results show that the obtained powder consists of a single phase orthorhombic structure with space group Pbnm. Optical performances of the sample have been investigated by excitation, emission and diffuse reflectance spectra for Zn²⁺ co-doped CaTiO₃:0.15Eu³⁺ nanophosphors. CaTiO₃:0.15Eu³⁺, 0.20Zn²⁺ nanophosphor revealed the intense red emission peek centred at 618 nm due to the hypersensitive ${}^{5}D_{0} \rightarrow {}^{7}F_{2}$ transition in Eu³⁺ under the excitation of 397nm UV-light. After the incorporation of Zn²⁺ into CaTiO₃:0.15Eu³⁺ the PL intensity have been remarkably enhanced by manifolds (5.5 times) in comparison to the intensity of $CaTiO_3:0.15Eu^{3+}$ nanophosphor. The ultra-violet visible (UV-vis) diffuse reflectance spectra has been carried out for the optical band gap calculation of the prepared sample. CCT value of optimized CaTiO₃: $0.15Eu^{3+}$, $0.20Zn^{2+}$ nanophosphor with CIE co-ordinate (0.59, 0.34) is found to be 2068 K. The experimental results reveals that the synthesized nanophosphors material Zn^{2+} co-doped CaTiO₃: $0.15Eu^{3+}$ can be used in solid state lighting devices.

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Time dependent morphological changes in Zinc Oxide powder and its effect on optical properties

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Zinc oxide (ZnO) is a direct band gap semiconductor. It is well known that chemical doping as well as intrinsic lattice defect greatly influences the electronic and optical properties of ZnO. Control of defect states is therefore key in achieving viable applications of ZnO. Visible optical properties such as photoluminescence can be tuned by introducing defects and change in morphology of ZnO nanostructures. In the present work ZnO a powder were prepared with different nanostructure by varying reactant NaOH concentration and was characterized by SEM, UV-Vis-NIR spectrophotometry, photoluminescence (PL) spectroscopy, and I-V measurements. After the characterization of the freshly prepared ZnO powders they were preserved for about 1.5 year in a vacuum desiccator and again characterized as mentioned above. We notice change in emission of colour from blue to bluish-white in photoluminescence spectra. The PL at blue region appears to be caused by energetic shifts of the valence band and/or the conduction band of ZnO. The change in colour emission is ascribed to the transitions between swallow and deep trap levels. Our results confirm, in spite of the fact that ZnO is a highly stable crystalline material over the time of varying environment condition introduces defect states and changes the morphology which vary the PL emission from blue to bluish-white.

Low-orange upconversion emission in Ho³⁺-doped NaZnPO₄ phosphors

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Rare earth (RE) doped upconversion (UC) luminescent materials have attracted researchers extensively due to their novel electric, magnetic and optical properties which have potential applications in different fields such as LEDs, temperature sensors, solar cells, fluorescent labels, optical telecommunication, biological applications, medical diagnostics, etc. [1-3]. Sodium zinc orthophosphate (NaZnPO₄) is a promising host material in the field of luminescence because of its low phonon frequency, high chemical, mechanical and thermal stability, etc. [4]. The Ho³⁺: NaZnPO₄ phosphors have been synthesized through conventional solid state reaction method. Frequency UC emission spectra upon 980 nm NIR CW diode laser excitation of the developed phosphors have been recorded at room temperature. From the UC emission spectra peaks are observed at ~ 545 nm, ~ 660 nm and ~ 757 nm corresponding to ${}^{5}F_{4}$, ${}^{5}S_{2} \rightarrow {}^{5}I_{8}$, and ${}^{5}F_{4}$, ${}^{5}S_{2} \rightarrow {}^{5}I_{7}$ transitions respectively. The generations of UC emission bands have been explained in detail by the suitable energy level diagram. The CIE colour coordinate of the prepared phosphors has been calculated at different pump powers which lie in the yellow-orange region. The experimental results suggest that the prepared material may be suitable in fabricating NIR to visible upconverter, display devices, etc.

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Synthesis, characterization and dielectric properties of PANI-

Fe-doped ZnO composite

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Polymer based organic and inorganic composite materials have received wide attention owing to their ease of synthesis, chemical stability and potential applications in diverse fields. Among the various conducting polymers with extended π -conjugated electron systems, such as polyaniline has been actively investigated by researchers in the last few decades because of its ease of synthesis, environmental stability, proton dopability, and unique optical properties. We prepared polyaniline (PANI)-Fe doped ZnO (inorganic) composites via in-situ polymerization of aniline with varying concentration of Fe doped ZnO nanoparticles. Polyaniline (PANI) was protonated with HCl to improve its electrical properties. The structural, optical, thermal and dielectric properties of the as-synthesized PANI@Fe doped ZnO composite were investigated. The fourier transform infra-red spectroscopy (FTIR), Xray diffraction (XRD), and energy dispersive X-Ray spectroscopy (EDX) results confirmed that the Fe:ZnO nanoparticles were successfully incorporated in PANI matrix. Scanning electron microscopy (FESEM) revealed the morphology of the as-prepared composite. The dielectric constant, dielectric loss and ac conductivity were studied using LCR meter in the frequency range 100Hz-5MHz. The optical properties were examined using UV-VIS spectroscopy in the wavelength range 200nm-800nm. The assembled of Fe doped ZnO nanoparticles on polyaniline surface and improved the thermal stability of the polyaniline structure in the temperature range 30°C-800°C.

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Synergistic Graphene Like MoS₂ Sheets/Conjugated Polymer Nano Composites for Supercapacitor Electrode Mandira Majumder¹, Ram Bilas Choudhary¹ and Anukul Kishor Thakur¹

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Supercapacitors, in today's world, proves to be very effective in meeting the ever-growing need for energy with various requisite properties such as high power density, a wide range of operating temperature, low cost, eco-friendliness, low maintenance, robustness, pollution free etc. However, it suffers from the disadvantage of low energy density as compared to the conventional batteries. A direct route to solve this problem is to come up with new electrode materials possessing high surface area, conductivity, chemical and thermal stability that will provide high energy density together with high power density and cyclic stability¹. By the virtue of its extraordinarily high surface area, graphene and its derivatives have attracted a great deal of attention of the researchers². MoS_2 is also a challenging material in this context, having a laminar structure analogous to graphene. Another class of materials, Conducting Polymers (CPs) such as Polypyrrole (PPY), Polyaniline (PANI). Polv (3.4)ethylenedioxythiophene) are widely researched on for their various interesting properties such as high charge density, low cost, ease of synthesis etc³. Though they suffer from thermal instability due to fragile backbone, incorporation of Carbon Nano Tubes (CNTs) seems to enhance the stability of polymers to a great extent⁴. We have studied the effect of incorporation of MoS₂ in a binary composite with PPY and a ternary composite with PANI-CNT. Composites were synthesized via. in-situ oxidative polymerization method. In both the cases, sp. capacitance was observed to enhance suggesting the positive effect of MoS_2 incorporation into the composites. This could be attributed solely to the graphene like laminar structure of MoS₂ that facilitates enhances surface area for ion exchange from the PPY and PANI-CNT chains to the electrolyte.

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Efficient NIR to blue upconversion emission in Tm^{3+} doped $Y_2\text{MoO}_6$ nanophosphors Manisha Mondal¹, Anita Kumari¹, Joydip Dutta¹ and Vineet K. Rai¹

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Lanthanide doped solid materials have taken much attention now a days due to their various applications in optical data storage, temperature sensing, optical amplifiers, LEDs, solar cells, biomedical applications, display devices etc. [1-3]. Lanthanide doped solid materials are attractive candidates for upconversion (UC) luminescence as they possess large number of energy levels and many of them are metastable in nature so they easily populated by infrared excitation sources. In the present work, thulium (Tm³⁺) doped yttrium molybdate (Y₂MoO₆) nanophosphors have been synthesized by solid state method. Among the various rare earth materials, thulium (Tm³⁺) is one of the most efficient rare earth ion used as dopant due to their strong blue and near infrared emissions and relatively weak red emissions [3]. The UC emission spectra have been recorded under 980 nm CW diode laser excitation in the 400-900 nm wavelength region at ~ 478 nm, ~ 650 nm and ~ 804 nm corresponding to the ¹G₄ \rightarrow ³H₆ transitions of Tm³⁺ ions respectively. Thus the prepared nanophosphors can be used efficiently in the fabrication of NIR to blue light upconvertors.

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Upconversion emission characterization of Ho³⁺/Ho³⁺-Yb³⁺ doped/codoped zinc tellurite glasses

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The Ho³⁺/Ho³⁺-Yb³⁺ doped/codoped TeO₂-ZnO glasses have been prepared by melting quenching method. The upconversion (UC) emission spectra for the Ho³⁺/Ho³⁺-Yb³⁺ doped/codoped zinc tellurite glasses have been recorded in the 400-800 nm wavelength range. A near infrared diode laser operating at 980 nm has been utilized to get the UC emission bands. In the case of Ho³⁺ doped glass only two UC emission bands are observed in the green and red region and assigned through the ${}^{5}F_{4}$, ${}^{5}S_{2}$ → ${}^{5}I_{8}$ and ${}^{5}F_{5}$ → ${}^{5}I_{8}$ transition, respectively of the Ho³⁺ ion. The effect of codoping with the Yb³⁺ ion is such that the UC emission intensity has been enhanced very much. Moreover, in the case of codoped glass, one extra UC emission bands is found in the NIR region and assigned by the ${}^{5}F_{4}$, ${}^{5}S_{2}$ → ${}^{5}I_{7}$ transition of the Ho³⁺ ion. The UC emission mechanisms for doped/codoped TeO₂-ZnO glasses have been discussed by using an energy level diagram. A detailed pump power study has been performed to obtain the number of photons involved in the UC emission bands. The calculated colour coordinates lying in the green region by using the CRI chromaticity diagram have been improved in the case of codoped glasses.

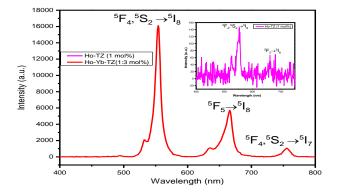


Figure: The UC emission spectra for the Ho^{3+} -Yb³⁺ codoped TeO₂-ZnO glass in the range of 400-800 nm. Inset shows the UC emission spectra for the Ho³⁺ doped TeO₂-ZnO glass in the range of 400-800 nm.

Microstructure Dependent Magnetic Domain Structures of Ni-C Nanocomposite Thin Films

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The present work envisages studies of magnetic domains of Ni-C nanocomposite thin films with varying microstructure. Experiments were performed on a couple of nanocomposite thin film samples designated as 21M and M/2, electrodeposited from nickel acetate solutions. Concentration of nickel acetate in the electrolytic solution was M and M/42 respectively for the above samples. All thin films were electrodeposited on ITO coated glass substrate for 20 minutes at 2.52 V with constant supply of current. Electrodeposited thin films were annealed at 80° C for 20 minutes. AFM study of 21M film reveals fine granular features while M/2 film shows the phenomenon of conglomeration of some granular particles which enhances the roughness of the film. Variation in microstructure was due to the change in concentration of nickel acetate in the electrolyte. Compositional analysis was performed by EDAX which shows the proportions of nickel and carbon in the at% ratio of nearly 1:4 in both films. It seems that after certain concentration of nickel acetate in the electrolyte no further deposition of nickel occurs on the substrate and hence proportions of nickel and carbon on the substrate saturate. Magnetic domain structures of both in plane magnetized Ni-C composite thin films were imaged with perpendicularly magnetized tip at room temperature in air. At 60 nm lift height both Ni-C thin films exhibit stripe domain pattern with continuous periodicity due to in plane magnetic moment and homogeneous distribution of nickel nanoparticles. 21M Ni-C composite thin film with homogeneously well-distributed fine granular morphological structure shows domain structure of smaller domain width in comparison of M/2 Ni-C composite thin film with unevenly distributed conglomerated granular and fine granular morphological structure.

Density functional study of charge transport properties of functionalized naphthalene

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A comparative theoretical study of the charge transport properties of naphthalene, substituted with F, Cl and CN using Density Functional Theory at B3LYP/6-311+G(d,p) computational level is reported. Several factors like; reorganization energy (λ), ionization potential (IP), electron affinity (EA), transfer integral (t) and mobility (μ) have been analyzed using Marcus theory (inner-sphere). It is observed that reorganization energy of the compound is getting reduced effectively and LUMO transfer integral, EA are found to be enhanced by cyanation rather than the fluorination or chlorination of naphthalene molecule inferring the enhancement of n-type characteristics in the compound, and therefore revealing its ambipolar nature.

Keywords: DFT, Marcus theory, reorganization energy, ionization potential, electron affinity, transfer integral, mobility.

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Electron induced ionization and Total cross section of Boron, Aluminum and Gallium trihalides

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Electron-molecule collision cross sections have been increasingly important for modeling and controlling discharge environments in low-temperature plasma reactors. Accurate inelastic and ionization cross section data are important for comprehending the mechanism of various chemical processes, which are required for modeling technical and fusion plasmas. Among various collision processes, electron-molecule collisions play a major role in plasma processing materials [1]. Processes of this kind, especially those involving metallic species, are of great interest in semiconductor manufacturing [2-4]. The interest in cross section data for boron, aluminium and gallium trihalides are due to their significance in low temperature plasmas, microelectronic industry and several other industrial plasma.

In the present work, total ionization cross section (Qion) data are computed for some important trihalides compounds of boron, aluminium and gallium with chemical formula XY3 (where X=B, Al and Ga and Y=F, Cl, Br and I) from the ionization threshold of the target to 5000 eV. Besides cross sections, we have also studied the correlation of maximum

ionization cross section with the square root of the ratio of polarizability to ionization potential for the molecules with known polarizabilities. A linear relation is observed between these quantities, confirming, the consistency of present method for evaluating cross section data. The present electron impact total ionization cross section for BF3 molecule is plotted in Figure 1. The nature and shape of the present cross section curve is similar to an old reported cross section by Kurepa et al. [5]. Their cross section is found to overestimate present values near the peak and beyond.

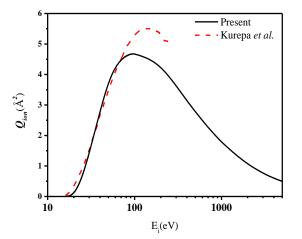


Figure 1. Q_{ion} of e-BF₃ scattering in Å². Solid line: present (O_{ion}): dashed line: Kurepa *et al*.

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PANI-PPy: ZnO hybrid nanocomposites for OLEDs applications: Fabrication and investigation of its optical and electrical properties

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Chemical oxidative polymerization technique was used for synthesis of PANI, PPy and its tertiary nanocomposites with ZnO of varying concentration. Their structure, optical and electrical properties were discussed. X-ray diffraction (XRD) and Fourier transform infrared spectroscopy (FTIR) were used to study the formation of polymer and its nanocomposites. Change in micro structural properties due to the incorporation of ZnO with varying concentrations was also studied. Field emission scanning electron microscope (FESEM) was used to study the surface morphology of pure PANI, PPy and its nanocomposites. Three characteristic bands at 420, 310 and 370 for the absorption of PANI, PPy and excitons of ZnO nanoparticles were observed using optical absorption spectrum. Band gap (E_g) was observed to be decreasing with the increase in ZnO concentration. Photoluminescence studies revealed the optimum intensity observed at 40% of tertiary nanocomposites and variation in blue emission (470 nm) was observed with the increase of the ZnO concentration. An enhance photocurrent density was calculated from I-V characteristics.

Keywords: Nanocomposites, Chemical oxidative polymerization, PL, AFM, I-V.

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Theoretical Investigation of Charge Transport Properties of Cyanated Pyrene Compound in Organic Semiconductor <u>Rudranarayan Khatua¹</u>, Smruti Ranjan Sahoo¹ and Sridhar Sahu¹

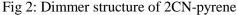
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We report the charge transport properties of cyanated pyrene (CN-pyrene) organic semiconductor by using computational density functional theory (DFT) method. The geometry has been optimized using B3LYP hybrid exchange-correlation functional and 6-311+G (d, p) level, with a fixed temperature of 300K. All the geometrical calculations were performed using the quantum chemistry software Gaussian09¹ and visualizing software Chemcraft. Along with the electron affinity (EA) and ionization potential (IP), the charge transport properties such as, reorganization energy (λ), transfer integral (t) and charge mobility (μ) were investigated. Further, the charge transfer rate has been calculated with the help of MLJ ((Marcus-Levich-Jortner) formalism². Though, we found a large value of the electron reorganization energy for 2CN-pyrene molecules as compared to hole reorganization energy; however, we noticed an increase of the electron affinity value by an amount of 0.48eV with the process of cyanation. Further, we found the maximum value of both hole and electron mobility as 2.82 cm²/V.sec and 3.02 cm²/V.sec, respectively for 2CN-pyrene molecules. However, with the ease of cyanation in the conjugated molecules, the electron mobility of 2CN-pyrene found to be enhanced by 0.84 cm²/V.sec from CN-pyrene. The increase of electron affinity and electron mobility may increase the n-type characteristics of 2CN-pyrene molecules.



Fig 1: Optimized structure of 2CN-pyrene



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Synthesis & Upconversion Emission Studies of Y_2O_3 : Tm³⁺/Yb³⁺ Phosphor Nanoparticles

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Tm³⁺/Yb³⁺ co-doped Y₂O₃ phosphor nanoparticles has been synthesized by the solution combustion technique using urea as fuel and reducing agent. The nitrate of rare earth Y(NO)₃.6H₂O, Yb(NO)₃.6H₂O and Tm(NO)₃.6H₂O are used in a schematic ratios to get the optimum emission. In order to investigate the annealing effect on upconversion emission the as prepared samples are further heated at 800 °C and 1000 °C. The phase formation of synthesized sample was carried out from XRD analysis. FTIR confirms the evolved impurities of nitrogen and water molecules, in addition to this the phonon frequency of host material are investigated as well. In order to analyse the surface morphology of prepared samples the FESEM images recorded. The controlled spherical shape and size of particle around 120 nm are monitored for sample annealed at 1000 °C. The comparative upconversion studies of these three powder samples (ASP, 800 °C and 1000 °C) are accomplished, subsequently, the improved emission intensity was found for the sample annealed at 1000 $^{\circ}$ C. The intense visible spectral band is observed at 478 nm. The emission has also been observed in the various spectral regimes after illuminating 976 nm diode laser. The upconversion spectra are recorded by a CCD spectrometer coupled with optical fiber. The CIE color diagram is plotted that confirms the sample is suitable for display devices and forensic science applications.

Nanopatterning of Zinc Oxide nanorod grating using thermal imprint lithography and hydrothermal technique Shefali Jayswal, Khusboo Jain and Rakesh S. Moirangthem

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We present here, non-conventional and cost effective nanofabrication method to periodically pattern zinc oxide nanorods by using thermal nanoimprint lithography and hydrothermal growth techniques. The fabrication process adopted in this work includes (1) patterning of 1D nanograting of aminopropyltriethoxysilane (APTES) on glass substrate using a PDMS stamp (replicated from DVD disc), (2) subsequent adsorption of ZnO nanoparticles on patterned nanograting, and (3) control growth of ZnO nanorods on patterned area. We believe that our fabricated ZnO nanostructure may have potential applications in the developments of electrochemical sensor, SERS substrate, solar cell, and display devices etc.

Nondestructive evaluation of ripening stage of Chiku (Manilkara zapota) using some numerical based Algorithms <u>Shubhashri Kumari</u>¹, and Anil Kumar Nirala²

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In the proposed work ripening stage of Climactric fruit Chiku (Manilkara zapota) has been evaluated nondestructively using laser speckle technique[1]. The biospeckle activity[2] inside the fruit has been evaluated qualitatively and quantitatively during its ripening stage using some numerical based algorithms. For qualitative analysis Co-occurence matrix (COM) as well as Inverse Fujii method and for quantitative analysis Inertia Moment (IM), Absolute value Difference (AVD) and Inverse Fujii methods have been used. The biospeckle activity has been found to increase during its ripening process. In addition Granulometric size distribution (GSD)[3] has been used for the first time for the evaluation of ripening stage of chiku and has been found that GSD value increased when the fruit is ripened.

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Study of activities of water at different conditions using Autoco-variance and Gray level co- occurence matrix method <u>Shubhashri Kumari</u>¹, and Anil Kumar Nirala²

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In the proposed work variations in activities of Water at diffrent conditions such as normal, chilled, hot with different temparature ranges and with alcohol has been evaluated using laser speckle technique. Laser speckle technique is a non - destructive, non - contact, non - invasive and easy technique[1]. The speckle size [2]and therefore activities have been evaluated using Autoco-variance method.Visual photographs along with corresponding speckle size has been found. Gray level co- occurence matrix (GLCM) has been used to differentitate the bruised and fresh region of an Indian apple[3]. In the proposed work GLCM has also been used to see the variations of activities at different condition of water. We conclude that Autocovariance method is a good speckle size estimator and GLCM method is found to be good analyzer in changes of water's textural parameters.

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Concentration Dependent Nanoindentation Study on Electrodeposited Nickel Incorporated Diamond like Carbon Thin Films

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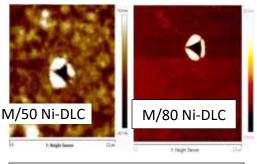
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The present work is based on the study of mechanical properties of nickel incorporated diamond like carbon (DLC) thin films by AFM nanoindentation. Mechanical properties of thin films are essential parameters for advanced devices. Thus, there has been an increasing interest to explore the mechanical and elastic properties of thin films. The nickel incorporated thin films were prepared by electrodeposition method. Molarity of nickel acetate were M/1050 and M/1680 in the electrolyte of two thin film samples designated as M/50 and M/80 Ni-DLC respectively. The films were synthesized on ITO coated glass substrates with voltage 2.5 V at room temperature for 35 minutes. They were annealed at 80°C for 20 minutes after deposition. The surface morphology and elemental composition of thin films were characterized by scanning electron microscopy (SEM) and EDAX respectively.

Indentations were performed with an applied load to examine the pressure induced deformation of the surface structure with Berkovich indenter. The applied load on nickel incorporated thin film was varied from $13.05\mu N$ to $65.25\mu N$. A typical load-displacement indentation curve was obtained. During loading, both elastic and plastic deformation occurs

under the indenter as the contact area changes with increasing depth. The area of the residual indentation in the sample was measured; the hardness is defined as the maximum load divided by the residual indentation area. Hardness of Ni-DLC film decreases with the increase of nickel concentration.

Acknowledgement: AFM nanoindentation was done at the SPM Laboratory, CRF, IIT (ISM), Dhanbad.



Indentations at load 65.25 µN

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Effect of attractive interaction on the structural behaviour of a system of Gay-Berne mesogens

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We have studied the effect of attractive forces on the isotropic-nematic and isotropic-smectic phase transitions in a system of axially symmetric long elongated molecules interacting via coarse-grained Gay-Berne intermolecular potential. An attractive parameter is introduced for describing the strength of attractive force. Pair correlation functions have been calculated by solving Percus-Yevick integral equation theory. These pair correlation functions are then used as structural inputs in the density functional theory to locate the freezing parameters. The effectiveness of the model is verified through comparison with the simulation results and with the results using traditional GB potential. We observe significant changes in the freezing parameters with the variation in the strength of attractive interaction between the molecules.

Integtral equation theory of nematic colloide <u>Biplab kumar Mandal</u> and Pankaj Mishra

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We have studied a system of spherical particle suspended in a nematic solvent confined in two dimensional plane. The particles are assumed to interact via a director distortion mediated interaction potential which varies as the nth power of the inverse interparticle separation. In experiments such a system of particles confined between two sheets of glass provide conditions for n to have values equal to 3, 5 or 7 depending upon the thickness of the space between the plates. Corresponding interactions are termed as dipoler, quadrupoler or octupolar respectively. In this presentation we have considered the case of quadrupolar and octupolar interactions and calculated the pair structures of the fluid using Roser-Young closure. We show our results of radial distribution functions and static structure factors and analyze their variation with interaction strength.

Phase behavior in binary mixture of nematic colloids: A density functional approach Anupam Kumar and Pankaj Mishra

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Density functional theory (DFT) of freezing has been used to investigate the topology of the phase diagram of systems of spherical colloidal particles dispersed in nematic liquid crystal (both one-component and two-component) confined to two-dimensional plane. The particles interact via nematic director deformation mediated elastic interaction potential [1, 2]. Depending upon the anchoring of nematic liquid crystal particles on the colloidal surface, we consider the effective potential to be (i) quadrupole-quadrupole or (ii) octupole-octupole. We have calculated the Pair-correlation functions used in DFT as input structural informations by solving the Roger-Young integral equation theory. Using the method of common-tangent construction we found stable triangular crystalline solid in the one-component system of both the cases. Considering the phase transition between fluid and disordered triangular solid, in the case of binary mixtures of quadrupoles, we found the temperature-composition phase diagram for highly symmetric mixture to be narrow spindle which changes to an azeotrope on increasing the asymmetry. On the other hand, for octupolar mixture the phase diagram is found to be spindle for highly symmetric case which phase separate on increasing the asymmetry.

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Study of Visible light driven Phtocatalysis of Rhodamine 6G dye with TiO₂ Microspheres

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Organic pollutants contained in the water are the major global problem that kills aquatic animals and its consumption by human being causes diseases and death. Water releases from textile industry present various toxic chemicals that are used for dying of textiles and remediation of the contaminated water is the biggest challenge. The destruction of the organic dyes contained in the water is also one of the problems which several researchers have attempted by utilizing metal oxide based semiconductor materials under illumination of light. In this work, we studied the photocatalytic efficiency of TiO_2 microspheres under sunlight illumination to degrade the Rhodamine 6G dye. Here, TiO₂ microspheres by a hydrothermal method having sizes around 5 micrometers and annealed at 450°C to get anatase phase. The prepared samples were characterized and analyzed using X-ray diffraction, Field emission scanning electron microscope, Energy dispersive X-ray spectroscopy, and UV-Visible spectrophotometer. The photocatalytic degradation of Rhodamine 6G dye in aqueous solution was monitored by employing TiO₂ microspheres as catalyst under sunlight illumination. The study was performed at different conditions i.e., a variation of pH, concentrations of the dye and amount of the catalyst present in the solution. Our experimental result as shown in figure 1 shows a complete degradation of the 16.5 µM Rhodamine 6G dye within 280 minutes under the sunlight illumination with 1 gm/L of TiO₂ powder in the aqueous dye solution. Hence, our prepared TiO₂ microspheres represent a promising cost-effective material for destruction of organic pollutants present in the water.

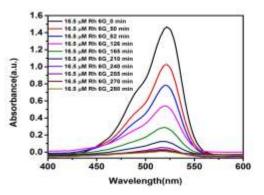


Figure - Degradation of Rhodamine 6G dye (16.5 µM) with 1gm/L of TiO₂ powder under sunlight.