Anexure-I

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Liquid crystal-nanocomposite materials for display and photovoltaic applications

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Executive Summary

Liquid crystal (LC) is an intermediate phase between solid and liquid which become an important area of research in the field of chemistry, physics, engineering and medical sciences. More and more advances in liquid crystal technology has led this multidisciplinary area to come with new LC based devices other than liquid crystal displays (LCDs), the most common application of liquid crystals. Since last decade liquid crystal research is not only focused on advanced LCDs but new devices such as spatial light modulators, 3D glasses, optical fibers and others have been developed. In addition to it, LCs has also being used in drug delivery and disease detection in medical field. Synthesis of new LC materials and new theories in LC physics has coupled to make it possible today to exploit LC in such different applications. This advanced scenario of LC could never be possible without using the non-mesogenic materials such as nanomaterials, dyes, polymers etc. to tune the properties of LC materials. Most recent studies on addition of nanoparticles have shown their importance to develop LCs in field of photo-voltaics and display applications.

The report contains research work on the effect of doped nanoparticles (NPs) on some liquid crystalline materials. The objective of the work was two fold: first is to understand that in what way different types of NPs and doped concentration of NPs affect the various properties of LCs. Second is to know precise concentrations of dispersed NPs necessary for its best utilization in different LC devices. Above this specific concentration the dispersed NPs starts degrading the performance of LCs properties rather than to improve it.

In the present report, studies of the LC-NPs composites have been pursued with two types of LC materials primarily nematic (N) phase (4'-octyl-4-cyanobiphenyl i.e. 8CB,4-pentyl-

4'-cyanobiphenyli,e.5CB) used in nematic LC displays and a second type forming columnar hexagonal (Col_{hex}) discotic phase (hexabutyloxytriphenylene ,HAT4) used in one dimensional conductors and photo voltaics . Three main types of NPs of different size have been used to dope in LC materials are gold, silver and barium titanate. In addition, Magnesium oxide nano particles have also been used. The report describes the change in the thermodynamical, optical, dielectric and electro-optical properties of liquid crystalline materials due to dispersion of NPs.

The thermodynamic study of the pure and dispersed materials has been carried out with the help of differential scanning calorimeter (DSC) of NETZSCH model DSC-200-F3-Maia which was operated at various scanning rates in the heating and cooling cycles. The change in the transition temperatures, enthalpies, entropies and transition width of different phases has been determined. Different phases have been identified by their optical textures observed under the polarizing light microscope (PLM) coupled with a hot stage (Instec, MK 1000). Temperature dependent dielectric studies of the materials have been carried out by the Newtons Phase Sensitive Multimeter (model PSM 1735 N4L) coupled with impedance Analysis Interface model IAI-1257 and Alpha-A high performance frequency analyzer from Nova Control technologies coupled with two-wire Impedance Interface ZG2. Temperature near the sample was determined by measuring thermo emf with the help of a six and half digit multi meter (Agilent model 34410A) with the accuracy of $\pm 0.1^{\circ}C$. Temperature and frequency dependent dielectric permittivity, loss and conductivity of different phases have been determined for the longitudinal and transverse geometry of the molecules from the measured capacitances (C) and resistances (R) in the frequency range from 1 Hz to 35 MHz. To analyze the measured dielectric data, complex dielectric permittivity (ε^*) has been fitted with the generalized Cole-Cole equation. For optical characterization UV-Vis absorbance spectra were recorded with Shimadzu UV

Spectrophotometer (UV-1800) in the wavelength region of 190-900 nm. Chloroform ($CHCl_3$) was used as a reference in a standard quartz cells with 10 mm path length. The energy band gap of pure and nanocomposites have been determined with the help of absorbance spectrum. Small angle X-ray scattering (SAXS) studies were carried out using an X-ray diffractometer (Rigaku, UltraX 18) operating at 50 kV and 80 mA current having Cu-Kα radiation of the wavelength of 1.54Å. The samples was filled in a capillary and then sealed. It was then heated to 100 °C and 120 °C giving exposure at these temperatures before going to isotropic liquid phase at 155 °C. The electro-optical studies of the nematic materials are performed by applying an AC voltage across the dielectric cell and transmission intensity of white light has been measured by a photo detector (made by Instec, USA) mounted on PLM and the corresponding photo- voltage has been measured with a six and half digit multimeter of Agilent. The threshold voltage, switching voltage and steepness of the transmission voltage curve have been determined for pure and its nanocomposites.

Further details can be seen in the following published papers

Papers Published in International Refereed Journals

1. Effect of the dispersed colloidal gold nanoparticles on the electrical properties of a columnar discotic liquid crystal. **Mukesh Mishra**, Sandeep Kumar, Ravindra Dhar. **RSC Adv. 2014**, 4, 62404-62412.

2. Electrical and electro-optical parameters of 4'-octyl-4-cyanobiphenyl nematic liquid crystal dispersed with gold and silver nanoparticles. **Mukesh Mishra**, Roman S. Dabrowski, Jagdish K. Vij, Avneesh Mishra, Ravindra Dhar. **Liq. Cryst. 2015**, 42, 15980-1590.

3. Thermodynamical, optical, electrical and electro-optical studies of a room temperature nematic liquid crystal 4-pentyl-4'- cyanobiphenyl dispersed with barium titanate nano

particles. **Mukesh Mishra**, Roman S. Dabrowski, Ravindra Dhar. **J. Mol. Liq. 2016**, 213, 247-254.

4. Gold nanoparticles in plastic columnar discotic liquid crystalline material. **Mukesh Mishra**, Sandeep Kumar, Ravindra Dhar. **Thermochimica Acta. 2016**, 631, 59-70.

5. Effect of High concentration of colloidal gold nanoparticles on the thermodynamic, optical and electrical properties of 2, 3, 6, 7, 10, 11-hexabutyloxytryphenylene discotic liquid crystalline material. **Mukesh Mishra**, Sandeep Kumar, Ravindra Dhar. **Soft Materials. 2017**, 15(1), 34-44

6. Thermodynamic study of a plastic columnar discotic material 2, 3, 6, 7, 10, 11-hexabutyloxytriphenylene (HAT4) dispersed with gold nanoparticles under elevated pressure. Pratibha Tripathi, **Mukesh Mishra**, Sandeep Kumar, Ravindra Dhar **J. Therm. Anal and Calorim. 2017,** 129, 315-322. DOI 10.1007/s10973-017-6128-4.

7. Thermodynamical, dielectric and electro-optical properties of a room temperature nematic liquid crystal 4-pentyl-4'-cyanobiphenyl dispersed with magnisium oxide nanoparticles (Under preparation). Now published as: Incorporation of magnesium oxide nanoparticle in to nematic liquid crystalline matrix, **Mukesh Mishra**, Rahul Uttam, Ravindra Dhar and Roman S Dabrowski, **Mol. Cryst. Liq. Cryst. 2020**, 708, 26-38.

Papers Presented in National/International Conferences

1. Influence of the dispersed colloidal Gold Nano Particles on the dielectric properties of a columnar discotic liquid crystal. **Mukesh Mishra***, Sandeep Kumar, Ravindra Dhar at 20th National Conference on Liquid crystals, Manipal University, Manipal, Karnataka from December 16-18, **2013**.
2. Discotic liquid crystal-nano composite: interplay with molecular dynamics

Mukesh Mishra*, Sandeep Kumar, Ravindra Dhar at XVI Annual Conference of International Academy of Physical Sciences, on Physical Sciences and Technology of Sustainable development at PDPM-IIIT-DM, Jabalpur, M.P. from March 20-22, **2014**.

3. Enhancement in the ionic conductivity of columnar discotic liquid crystal – gold nano composites. **Mukesh Mishra***, Sandeep Kumar, Ravindra Dhar at International Conference on Advance Material & Applications, Centre of Material Sciences, IIDS, University of Allahabad from March 24-26, **2014**.
4. Influence of low concentration gold nanoparticles on the electrical parameters of a discotic liquid crystal. **Mukesh Mishra***, Sandeep Kumar, Ravindra Dhar at International workshop on materials, Lucknow University, Lucknow July 15, **2014.**
5. Thermodynamical, optical and dielectric studies of the (2, 3, 6, 7, 10, 11)-Hexabutyloxytryphenylene (HAT4)-gold nanoparticle composites. **Mukesh Mishra***, Sandeep Kumar, RavindraDhar at 21st National Conferences on Liquid Crystals, V.S.S.D.P.G. Kanpur from December 16-18, **2014.**
6. Induction of plasmonic resonance and enhancement of the electrical conductivity in the columnar mesophase of discotic liquid crystalline material. **Mukesh Mishra***, Sandeep Kumar, RavindraDhar at International conference on Light Quanta: Modern Perspective and Applications, Allahabad University, Allahabad, on December, 14-16-8, **2015**.
7. Electrical and electroptical parameters of 4 octyl-4-cyanobiphenyle nematic liquid crystal dispersed with gold and silver nanoparticles. **Mukesh Mishra***, Roman S. Dabrowski, J. K. Vij, RavindraDhar at 22nd National conference on liquid crystal, DIT University, Dehradun, on December, 21-23, **2015**.

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