Study of Electro-Optics of Anisotropic Molecules for Photonics Applications

Summary of the Thesis

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Submitted By
Pawan Singh
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Under the supervision of
Dr. Khem Bahadur Thapa

Department of Applied Physics
School for Physical Sciences
Babasaheb Bhimrao Ambedkar University
(A Central University)
Lucknow -226025, U.P. (India)

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Summary

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In nature, three kinds of matter exist solid, liquid, and gas. Although the different kinds of matters have intensive or extensive properties they transformed into one another by changing the external fields and thermodynamic conditions. For example, water shows all three phases of matter, it is converted into gas by supplying heat and also solidified via taking out heat or cooling it. The condensed materials exhibit into different types depending on the order of molecules or crystalline nature. The condensed materials could be isotropic or anisotropic depending on the molecular properties. Isotropic materials have direction independent dielectric and optical characteristics i.e. the isotropic materials show the same dielectric constant in different directions while the anisotropic materials have direction-dependent dielectric properties, optical characteristics, and dispersion relations [1,2].

The anisotropic materials have anisotropy that may be in dielectric properties or optical properties and such materials changes their optical properties by changing electric fields and temperatures. Depending on the interaction of the normal surface of the ellipsoid index with xz plane, the anisotropic materials may be uniaxial or biaxial. There are different examples of anisotropic materials, some are found in nature e.g. ice, quartz, and some could be synthesized in laboraties, e.g. $LiNbO_3$, $BaTiO_3$, Liquid Crystals, and so on. Generally, liquid crystal (LC) is organic benzene derived material and it is an intermediate state between pure liquid phase and solid crystal phase. LCs exhibit liquid-like characteristics as well as crystal-like characteristics, which are dependent on intensive properties. The applications of electric field or voltage in the liquid crystals show orientation and reorientation of their molecules, and such properties of LCs are very useful to design electro-optical properties due to change in the intensive properties. LCs have mainly three types: lyotropic, polymeric, and thermotropic and types of LCs are depending on the shape, size, order of molecules as well as temperature. The thermotropic LCs exhibits different phases like nematic,

cholesteric, smectic phases [3-7]. To design the tunable devices, the nematic and cholesteric phases of LC are widely studied.

In my research work, we have used the nematic liquid crystal (NLC) as defect materials in a one-dimensional periodic structure (1-DPS) of dielectric materials and studied the tuanble optical properties of 1-DPS with defect LC materials.

The multilayered periodic structures are generally known as photonic crystals (PCs) having periodic modulation of dielectric functions in different dimensions which exhibits photonic band gaps (PBGs) in the resultant transmission. The different types of PCs are classified into one-dimensional photonic crystals (1-DPCs), two-dimensional photonic crystals (2-DPCs), and three-dimensional photonic crystals (3-DPCs) [8-11]. The idea to control electromagnetic radiation in periodic media was described by Yablonovitch and John. [12,13]. The idea of controlling the tunable transmission of electromagnetic in periodic layered media or PCs with LCs was given by Busch et al. [14] and experimentally confirmed by Yoshino et al. [15]. Using LC as defect layers in periodic layers, the tunability of PCs could be achieved which was suggested by various scientists [16-42]. By controlling the optical parameters of LCs like orientation, twisting, nonlinearity, temperature, and so on, all-optical characteristics of LC embedded PCs could be achieved to use in optoelectronics, photonics, and electro-optical devices.

The thesis work is divided into six chapters and the chapter-wise study is given in the following sections.

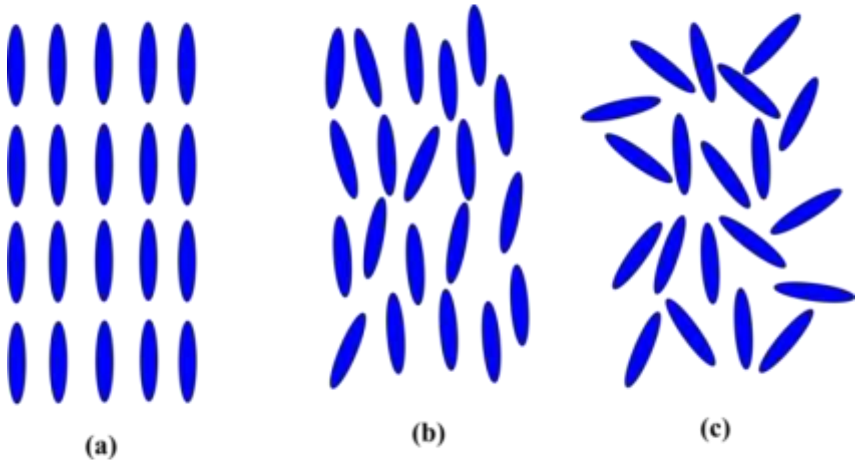

Figure 1: The phase of crystal: (a) pure crystalline phase, (b) liquid crystal phase, (c) pure liquid phase.

Chapter 1 describes the electro-optics of anisotropic materials as well as liquid crystals. The ellipsoid index of anisotropic molecules changes with the electric field and voltages. The anisotropic LC is an intermediate phase between liquid and solid as shown in figure 1. LC changes its optical properties when an electromagnetic wave interacted with the molecules. When electromagnetic waves interact with LC, the molecules orient depending on the threshold intensity of the wave, known as the Freedericksz transition [43]. The nematic phase of LCs shows three different types of molecular configurations: splay, bend, and twist.

In nematic liquid crystals (NLCs), the molecules orient in-plane but the molecules show unwinding of the helical pattern of the molecules with a certain pitch for cholesteric liquid crystals (CLCs). The pitch of CLCs changes with the application of electric and magnetic fields and for a sufficiently high field, the helical patterns show unwinding resulting all molecules are oriented in the applied field directions [3,7]. Another phase of LC, the Smectic phase has complicated optics and formulations depending on the molecular pattern of the LCs. To fabricate the nonlinear tunable photonic devices, nematic and cholesteric liquid crystals are very useful materials with periodic structures. The optical characteristics of such periodic structures / PCs are used to study mainly four methods: plane wave expansion (PWE) method, finite element method (FEM), finite difference time domain method (FDTD), and transfer matrix method (TMM) [44-47]. Besides this, FIT and BPM are also used to study the optical characteristics of PCs. The literature survey provides the highlights of the discovery of liquid crystals and the schematic investigation of liquid crystals in various tunable photonic devices. Based on the bistable properties of liquid crystals, the optical properties of liquid crystals as defect layers in 1-DPS of dielectric materials with anisotropic materials were also discussed.

In chapter 2, theory and mathematical formulation to investigate the transmission characteristics of PCs embedded with anisotropic materials are summarized. The mathematical formulations based on Maxwell's equations are derived, which gives the transmission and absorption characteristics of 1-DPCs considering TE and TM polarization modes [48-50]. In the whole thesis work, TMM is considered to investigate the optical properties of 1-DPS of dielectric materials with LCs, graphene, $LiNbO_3$, and nano-composite materials with a variety of different parameters.

Chapter 3 gives the tunable transmission properties of 1-DPS of glass and Si materials with a PAA NLC defect embedded with graphene layers at different orientation angles of LC molecules. The interaction of EMW with NLC is investigated for increasing and decreasing the intensity of the wave. A nonlinear differential equation for LC orientation has been solved with the help of Dirichlet boundary conditions. The obtained results suggest that the molecules of LC show orientation when the intensity of EMW is reached to threshold value and the molecules are gained the maximum value in the middle of the LC layer. For the increasing and decreasing intensity of EMW, the molecules follow the dissimilar paths for orientation and reorientation of molecules, and the hysteresis loop for PAA NLC is shown in figure 2. The nature of the hysteresis loop is also obtained in the transmission which reveals that the orientation and reorientation of molecules of the LCs are affected the optical properties.

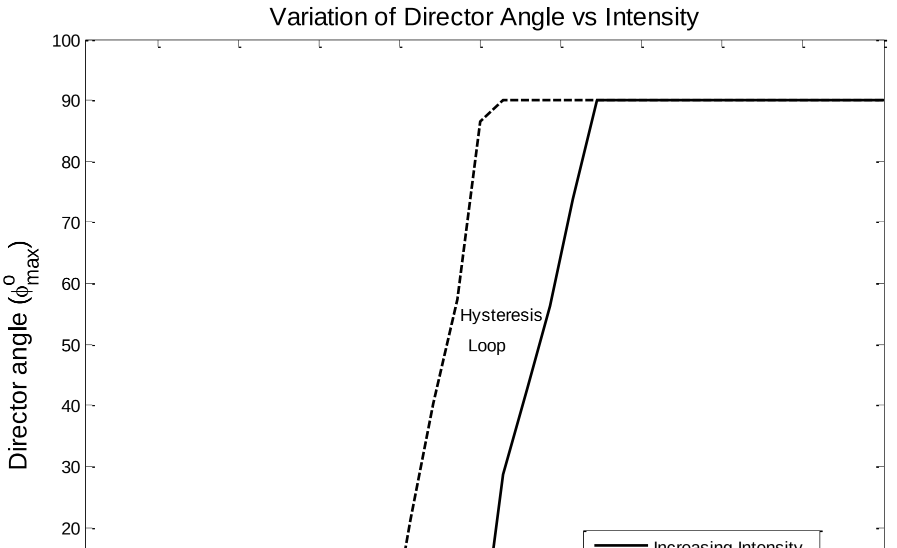

Figure 2: Maximum values of liquid crystal director (ϕ^{0}_{max}) versus intensity ratio (I/I_{Fr}) for increasing and decreasing intensity.

To apply the TMM for calculating the transmittance, the dielectric tensor of LC must be diagonalized for 0^o and 90^o director angles [51]. The transmission properties of the proposed structure at three director angles of the LC are shown in figure 3. As the director angle of LC increases, the defect modes in the PBG region are shifted to higher wavelengths. The different wavelengths are shown hysteresis loops due to the Freedericksz transition in LC which affects the transmittances. The difference between the defect mode transmissions for considered director angles has remained almost uniform, but it is shifted to lower wavelength regions with incident angles. The orientation of the LC molecules in the defect layer tunes the sharp defect mode in the PBG region of considered 1-DPS with the NLC defect layer [63]. This study shows that the propagation of EMW in NLC led to switching characteristics due to the molecular orientation inside the LC cell and it may be very fascinating to study the use of optical switching in photonic devices.

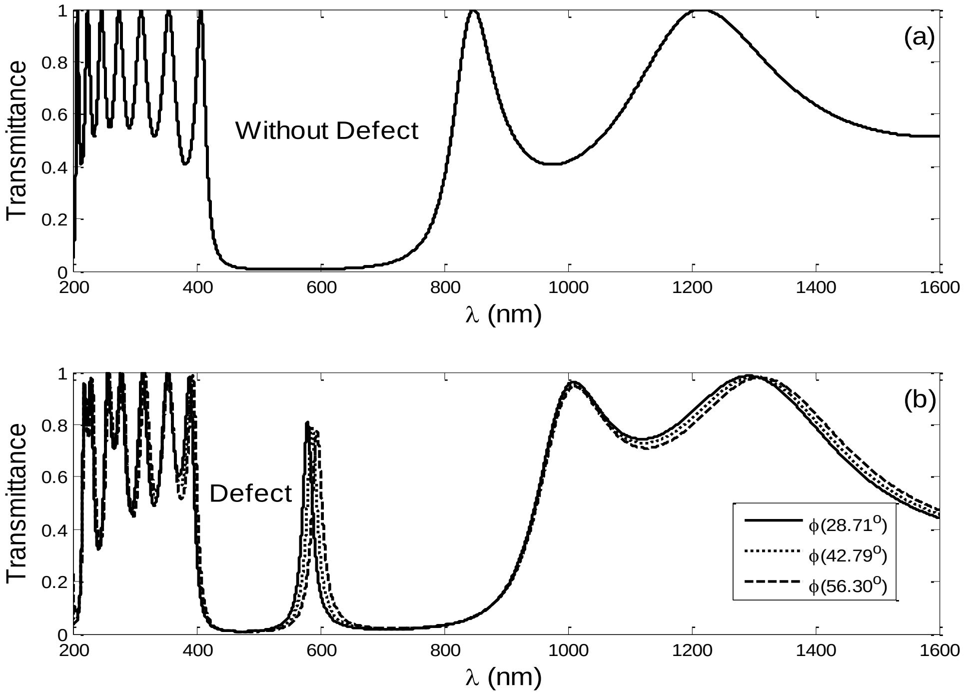

Figure 3: Comparative transmissions of 1-DPS without and with the NLC defect at different molecular orientation angles.

The behavior of the LC orientation angle is changed according to the intensity of electromagnetic wave and the threshold value. Due to such orientation-dependent property of LC, a tunable transmission of 1-DPS is obtained with the NLC defect layer in the periodic structure. As the orientation angle of LC changes, the defect transmission peaks are shifted to higher wavelengths. Such 1-DPS with defect LCs may help to design all-optical tunable devices with a controlled orientation angle of the molecules by induced transition in LC layer.

Similarly, we have studied absorption characteristics of 1-DPS of dielectric materials with NLC defect material embedded with graphene layers and showed high absorption due to the imaginary nature of graphene [52]. The transmittances of defect modes peaks in PBG are found 13%, 12%, and 11% for LC 28.7^o, 42.7^o, and 56.3^o orientation angles, respectively. The proposed 1-DPS containing LC with and without graphene layers have the configurations as $(Si/glass)^m/NLC/(Si/glass)^n$, $(Si/glass)^m/G/NLC/G/(Si/glass)^n$ with m=n=3 and the optical properties of such 1-DPS at three different director angles were studied. The proposed 1-DPS with NLC embedded graphene layers shows the absorption of defect peaks in the PBG region. With higher periodicity of dielectric materials in 1-DPS containing LC with graphene, the absorption characteristics also show unusual characteristics with the incident angle for TM mode. As the periodicity of binary layers in 1-DPS changes as m=3, n=5, the absorption of defect peaks is enhanced in the PBG region. Such enhanced absorption of defect peaks may be useful to design optical sensors, absorbers, etc. depending on the periodicity of layers, chemical potential of graphene, and orientation of LC molecules.

Chapter 4 illustrates the transmission properties of 1-DPS of TiO_2 and SiO_2 materials with a sandwich of $LiNbO_3$ with E7 LC at a different voltage, temperature, and incident angle of EMW. The dielectric properties of E7 LC are dependent on the temperature and followed the same dielectric indices at the transition / clearing temperature of LC. The ordinary dielectric constant of anisotropic material $LiNbO_3$ is dependent on the applied voltage while the extraordinary constant is dependent on the incident angle as well as the applied voltage [53].

The dielectric or refractive indices (n_e, n_o) and electro-optical parameters (r_{13}, r_{33}) of $LiNbO_3$ in the absence of an electric field are 2.20, and 2.70 and are $9.6pmV^{-1}$, $30.9pmV^{-1}$ respectively. The behavior of refractive indices of electro-optical material $LiNbO_3$ with a voltage range of -200V to 200V at 0^o, 30^o, 45^o incident angles is revealed in figure 4. The proposed 1-DPS consisting of as defect anisotropic materials E7 LC and LNO may be used in tunable photonic and optoelectronic devices like optical switches, filters, modulators, wavelength selectors, etc. As discussed earlier, the voltage-dependent refractive indices of $LiNbO_3$ have tuned the obtained defect modes in the transmission of 1-DPS $(SiO_2/TiO_2)^5/LC/LNO/LC/(TiO_2/SiO_2)^5$; therefore, we have analyzed the transmissions of 1-DPS at different voltages; -200V, 0V, and 200V considering TE and TM polarizations.

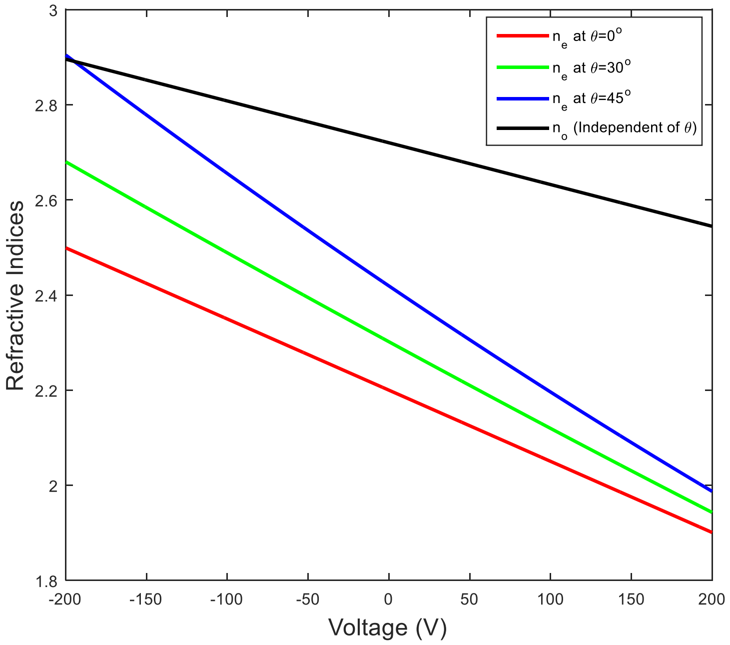

Figure 4: Deviation of refractive indices (n_e, n_o) of $LiNbO_3$ with voltage (-200V to 200V) at 0^o, 30^o, 45^oincident angles.

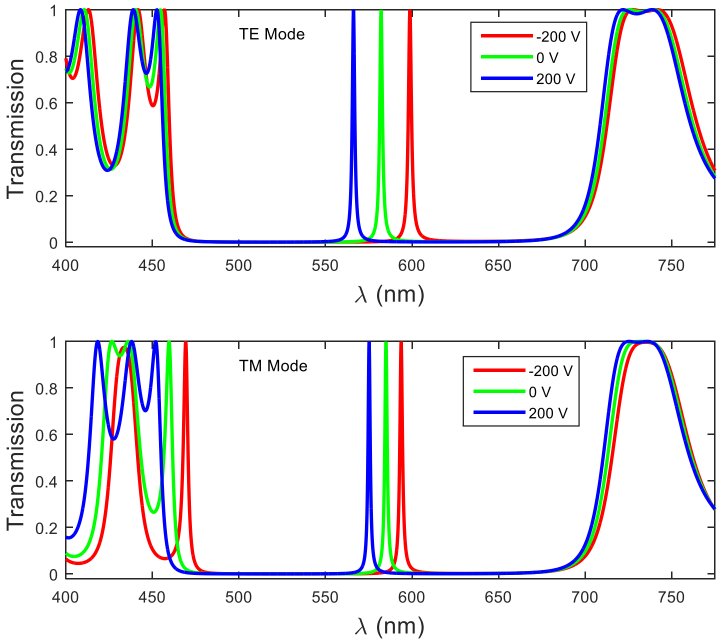

Figure 5: Transmission of 1-DPS $(SiO_2/TiO_2)^5$/LC/LNO/LC/$(TiO_2/SiO_2)^5$ at -200V, 0V, 200V voltages considering TE and TM polarizations.

The optical transmissions of 1-DPS at -200V, 0V, and 200V voltages for TE and TM modes are represented in figure 5. The defect transmission peaks in the PBG region are shifted toward the lower and longer wavelength for positive and negative biasing voltages on the LNO material, and such shifting of defect modes is higher for TE polarization than TM polarization. Such shifting of defect modes may very useful in designing of the optical switch with the variation of voltages.

The transmission of 1-DPS for both polarization modes is studied at 300K, 330K, 360K temperature when applied voltage is 0V. The study suggests that the transmission of 1-DPS and defect mode transmission are effectively varied for the TM polarization than the TE polarization. The wavelength of defect mode transmissions in PBG for TE polarization is 582.1nm, 585.9nm 584.7nm at 300K, 330K, 360K temperatures, respectively. Based on calculated results, we can fabricate temperature and voltage-dependent optical switches. By controlling the temperature and dielectric constant of LCs, the whole optical properties of 1-DPS with a sandwich of $LiNbO_3$ with E7 LC also can be varied. Hence, temperature-based sensors or switches of considered 1-DPS containing defect layer of $LiNbO_3$ material embedded with E7 LC may be designed with the variation of voltages.

The transmission of 1-DPS with a sandwich of $LiNbO_3$ with E7 LC is studied at 0^o, $30^{o,}$ and 45^o incident angles for 0V and the wavelengths of defect mode transmission in the PBG region for TE polarization are found 582.2nm, 568.8nm and 554.7nm for 0^0, 30^0, and 45^0 incident angles, respectively. Similarly, the wavelengths of defect mode transmission for TM polarization are found 585nm, 564nm, and 543nm for same incident angles. The location of defect mode transmissions varies with the incident angle of EMW and a tunable omnidirectional PBG may also be achieved with such 1-DPS at different voltages for various photonic applications.

Chapter 5 explains the dielectric function of the nanocomposite structure of E7 LC and spherical silver nanoparticles (Ag-NPs) at different radii and filling fractions of nanoparticles and the temperature of LC. Using the Maxwell-Garnett Model, the effective dielectric function of the proposed nano-composite structure is calculated [54, 55]. The effective dielectric function of NC is given as; $\varepsilon_{eff} = \frac{2\varepsilon_{LC} f(\varepsilon_m - \varepsilon_{LC}) + \varepsilon_{LC}(\varepsilon_m + 2\varepsilon_{LC})}{2\varepsilon_{LC} + \varepsilon_m + f(\varepsilon_{LC} - \varepsilon_m)}$; where ε_{LC} = dielectric function of LC, ε_m =

dielectric permittivity, and f=filling fraction of Ag-NPs in the host LC. The ε_m of the spherical Ag-NPs is calculated with the Drude model that is $\varepsilon_m = \varepsilon_0 - \frac{\omega_p^{\ 2}}{\omega^2 + i\omega\eta}$, where ω_p = plasmon frequency, ε_0 = relative dielectric permittivity, and η = damping frequency of Ag-NPs. The damping frequency is dependent on the Ag-NP size and the electron velocity (ν_f) at Fermi-energy is given by; $\eta(r) = \eta_0 + \frac{\nu_f}{r}$, where η_0 = decay constant acquired by electrons through electron-phonon and electron-electron scatterings etc.

The effective dielectric function of the NC is designed with E7 LC and spherical NPs of 5nm radius with varying filling fractions (f) in NC. In designing of NC, the plasmon frequency ω_p and decay constant for spherical Ag-NPs are taken as $2\pi \times 2.17 \times 10^{15}\,\mathrm{Hz}$ and $2p\ ´\ 4.8\ ´\ 10^{12}\,\mathrm{Hz}$ respectively with $\varepsilon_0 = 5$ [47-49].

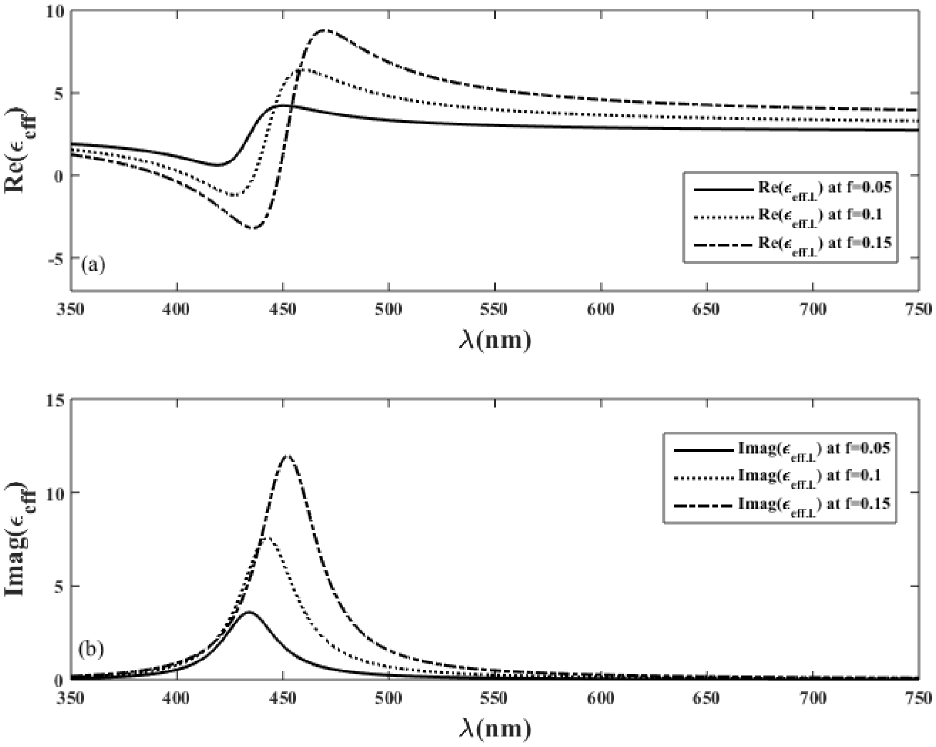

Figure 6: Variation of real and imaginary parts of the perpendicular component of effective dielectric functions of NC at the filling fraction: 0.05, 0.10, and 0.15.

The filling fraction (f) modifies the dielectric function of NC and attains higher values at a higher filling fraction as shown in figures 6 and 7.

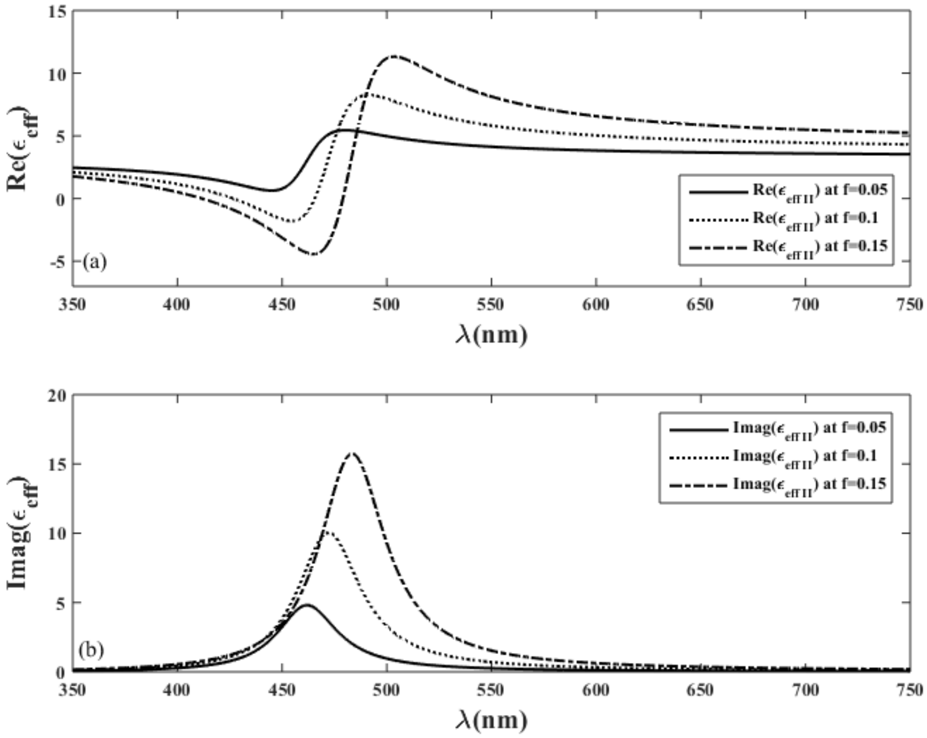

Figure 7: Variation of real and imaginary parts of the parallel component of effective dielectric functions of NC at the filling fraction: 0.05, 0.10, and 0.15.

The real parts of the perpendicular and parallel component of effective dielectric function first decreases and then increases with increases the wavelength, while the imaginary part of the perpendicular and parallel component of effective dielectric function also increases and then also decreases as shown in figures 6 and 7. We have also studied these dielectric functions with the variation of the radius where the values of both parts are increased with increases the radius of nanoparticles in the NC considering 0^{o} and 90^{o} orientations of molecules. A variation in both parts of effective dielectric functions of NC for 350nm to 550nm wavelength region is found. The observed results suggest that the surface plasmon resonance (SPR) is also related to the molecular orientation of E7 LC which is adjusted to the effective dielectric index of NC with Ag-NPs. By study the SPR, the interaction of Ag-NPs with LC also can be investigated fundamentally.

To study the effect of size and filling fraction of NPs, the transmission properties of 1-DPS of TiO_2 and SiO_2 materials with NC defect layer, $(TiO_2|SiO_2)^m|NC|(TiO_2|SiO_2)^m$ with m=5, 3, figure 8, have been calculated by transfer matrix method (TMM) [43].

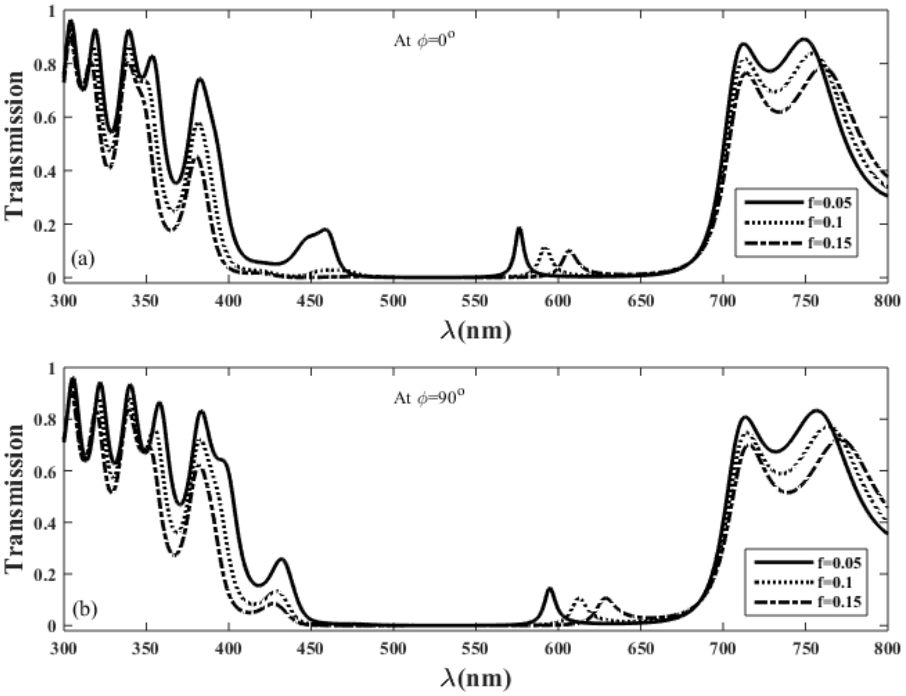

Figure 8: Transmission properties of 1-DPS with NC at 0.05, 0.10, and 0.15 filling fractions of Ag-NPs for (a) $\phi = 0^o$ and (b) $\phi = 90^o$.

The considered 1-DPS also shows the absorption properties due to silver nanoparticles which supports the surface plasmon resonance (SPR) effect in the material as shown in figure 9.

As the radius of Ag-NPs increases, the effective dielectric permittivity of NC and the corresponding SPR increase due to the decreasing scattering rate of conduction electrons. The whole optical properties of 1-DPS are tuned with size variation of NPs which considerably alters the dielectric response of the defect NC layer.

The optical properties of NC significantly change with the variation of the parameters of the guest (Ag-NPs) and host materials (E7 LC). The dielectric function of NC is associated with surface plasmon resonance (SPR) which affects the optical properties of NC and hence a defect layer of NC in 1-DPS gives the tunable transmission at different parameters of NC interconnected with variation in the SPR. The designed 1-DPS may be used as tunable bistable optical devices at different filling fractions and radii of Ag-NPs.

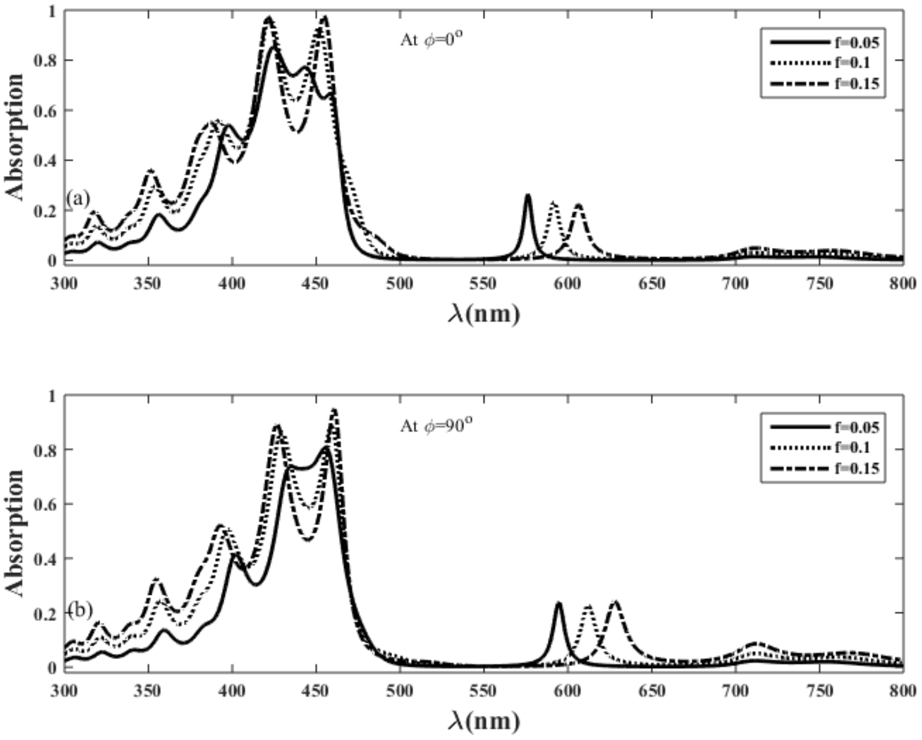

Figure 9: Absorption properties of 1-DPS with NC at 0.05, 0.10, and 0.15 filling fractions of Ag-NPs for (a) $\phi = 0^{o}$ and (b) $\phi = 90^{o}$.

Chapter 6 gives brief conclusions and future prospects of the thesis. This chapter discusses the basic idea of the applications of anisotropic molecules of various LCs, with LNO and graphene materials in the field of photonics, spintronics, and quantum computers.

References

[1] A. Yariv, P. Yeh, *Optical Waves in Crystals: Propagation and Control of Laser Radiation*, John Wiley and Sons, USA, 1984.

[2] P. Yeh, C. Gu, *Optics of Liquid Crystal Display*, John Wiley and Sons, USA, 1999.

[3] P. G. deGennes, *The Physics of Liquid Crystals*, Clarendon Press Oxford, 1974.

[4] S. Chandrasekhar, *Liquid Crystals*, Cambridge: Cambridge University Press, 1992.

[5] A. Ciferri, A., W. R. Krigbaum, and R. B. Meyer, *Polymer Liquid Crystals*, Academic Press., New York, 1982.

[6] L. M. Blinov, and V. G. Chigrinov, *Electrooptic Effects in Liquid Crystal Materials*, Springer-Verlag, New York 1994.

[7] I. C. Khoo, *Liquid Crystals*, John Wiley and Sons, New Jersey, 2007.

[8] J. D. Joannopoulos, R. D. Meade, and J. N. Winn, *Photonic Crystals: Molding the Flow of Electromagnetic wave*, Princeton, Princeton Univ. Press, 1995.

[9] M. Skorobogatiy, and J. Yang, *Fundamentals of Photonic Crystal Guiding*, New York, Cambridge University Press, 2009.

[10] I. A. Sukhoivanov, and I. V. Guryev, *Physics and Practical Modeling*, Berlin, Springer, 2009.

[11] K. Sakoda, *Optical Properties of Photonic Crystals*, New York, Springer, 2005.

[12] E. Yablonovitch, Inhibited spontaneous emission in solid –state physics and electronics, *Phys. Rev. Letts.*, 58, 2059-2062, 1987.

[13] S. John, Strong localization of photons in certain in disordered dielectric superlattices, *Phys. Rev. Letts*, 58, 2486-2489, 1987.

[14] K. Busch and S. John, Liquid-Crystal Photonic-Band-Gap Materials: The Tunable Electromagnetic Vacuum, *Phys. Rev. Letts*., 83, 967-970, 1999.

[15] K. Yoshino, Y. Shimoda , K. Nakayama , T. Tamura , T. Matsui , H. Kajii and M. Ozaki, Novel Electrical and Optical Properties of Liquid Crystals Infiltrated in Opal as Photonic Crystal, Molecular Crystals and Liquid Crystals Science

and Technology. Section A. *Molecular Crystals and Liquid Crystals*, 364, 501-509, 2001.

[16] M. Foresti, Plane-wave propagation in a plane-oriented nematic liquid-crystal multilayer: the case of a wave incident upon the plane containing the liquid-crystal directors, *J. Opt. Soc. Am. A*, 6, 1254-1259, 1989.

[17] R. C. Sharp, D. P. Resler, D. S. Hobbs, and T. A. Dorschner, Electrically tunable liquid-crystal wave plate in the infrared, *Opt. Letts.*, 15, 87-89, 1990.

[18] Y.-C.Yang, C.-S. Kee, J.-E. Kim, and H. Y. Park, J.-C. Lee, Y.-J. Jeon, Defect modes of cholesteric liquid crystals, *Phys. Rev. E*, 60, 6852-6854, 1999.

[19] S. W. Leonard, J. P. Mondia, H. M. van Driel, O. Toader, and S. John, K. Busch, A. Birner and U. Gosele, V. Lehmann, Tunable two-dimensional photonic crystals using liquid-crystal infiltration, *Phys. Rev. B*, 61, R2389-R2392, 2000.

[20] D. Kang, J. E. Maclennan, N. A. Clark, A. A. Zakhidov, and R. H. Baughman, Electro-optic Behavior of Liquid-Crystal-Filled Silica Opal Photonic Crystals: Effect of Liquid-Crystal Alignment, *Phys. Rev. Letts.,* 86, 4052-4055, 2001.

[21] C.-S. Kee and H. Lim, Two-dimensional tunable metallic photonic crystals infiltrated with liquid crystals, *Phys. Rev. B*, 64, 085114(1-7), 2001.

[22] H. Takeda and K. Yoshino, Disappearances of uncoupled modes in two-dimensional photonic and crystals due to anisotropies of liquid crystals, *Phys. Rev. E*, 67, 056612(1-5), 2003.

[23] R. Ozaki, H. Miyoshi, M. Ozaki, and K. Yoshino, Fast Electrooptic Response Based on Defect Mode Switching in One-Dimensional Photonic CrystalContainingNematic Liquid Crystal and Ferroelectric Liquid Crystal as a Defect Layer *Ferroelectrics*, 312, 63–69, 2004.

[24] R. Ozaki, M. Ozaki And K. Yoshino, Defect Mode in One-Dimensional Photonic Crystal with In-Plane Switchable Nematic Liquid Crystal Defect Layer, *Jpn. J. Appl. Phys.*, 43, L1477-L1479, 2004.

[25] J.-Y. Chen and L.-W. Chen, Defect modes in a stacked structure of chiral photonic crystals, *Phys. Rev. E*, 71, 061708(1-7), 2005.

[26] E. Graugnard, J. S. King, S. Jain, and C. J. Summers, Y. Zhang-Williams and I. C. Khoo, Electric-field tuning of the Bragg peak in large-pore TiO_2 inverse shell opals, *Phys. Rev. B*, 72, 233105(1-4), 2005.

[27] R. Ozaki, Y. Matsuhisa , M. Ozaki & K. Yoshino, Laser Action Based on Electrically Controllable Defect Mode in One-Dimensional Photonic Crystal Containing Conducting Polymer and Liquid Crystal Defect Layers, *Mol. Cryst. Liq. Cryst.*, 433, 237-245, 2005.

[28] R. Ozaki , Y. Matsuhisa , M. Ozaki and K. Yoshino (2005) Low Driving Voltage Tunable Laser Based on One-dimensional Photonic Crystal Containing Liquid Crystal Defect Layer, *Mol. Cryst. Liq. Cryst.*, 441, 87-95, 2005.

[29] C.-Y. Liu and L.-W. Chen, Tunable band gap in a photonic crystal modulated by a nematic liquid crystal, *Phys. Rev. B*, 72, 045133(1-5), 2005.

[30] R. Ozaki , H. Miyoshi , M. Ozaki and K. Yoshino, Tunable Defect Mode in One-Dimensional Photonic Crystal with Liquid Crystal Defect Layer, *Mol. Cryst. Liq. Cryst.*, 433, 247-257, 2005.

[31] P. Halevi and J. A. R.-Avendaño, J. A. R.-Cervantes, Electrically tuned phase transition and band structure in a liquid-crystal-infilled photonic crystal, *Phys. Rev. E*, 73, 040701(1-4), 2006.

[32] S. Gottardo, M. Burresi, F. Geobaldo, L. Pallavidino, F. Giorgis, and D. S. Wiersma, Self-alignment of liquid crystals in three-dimensional photonic crystals, *Phys. Rev. E*, 74, 040702(1-4), 2006.

[33] I. H. Bechtold, F. Batalioto, L. T. Thieghi, B. S. L. Honda, M. Pojar, J. Schoenmaker, A. D. Santos, V. Zucolotto, D. T. Balogh, O. N. Oliveira, Jr., and E. A. Oliveira, Transitions in the orientational order of liquid crystals induced by periodic patterned substrates, *Phys. Rev. E*, 74, 021714(1-6), 2006.

[34] A. E. Miroshnichenko, I. Pinkevych, and Y. S. Kivshar, Tunable all-optical switching in periodic structures with liquid-crystal defects, *Opt. Exp.*, 14, 2839-2844, 2006.

[35] R. Ozaki, H. Moritake, K. Yoshino, and M. Ozaki , Analysis of defect mode switching response in one-dimensional photonic crystal with a nematic liquid crystal defect layer, *J. Appl. Phys*., 101, 033503(1-6), 2007.

[36] A. H. Gevorgyan and M. Z. Harutyunyan , Chiral photonic crystals with an anisotropic defect layer, *Phys. Rev. E*, 76, 031701(1-9), 2007.

[37] J. A. Reyes, J.A. R.-Avendano, P. Halevi , Electrical tuning of photonic crystals infilled with liquid crystals, *Opt. Commun*., 281, 2535-2547, 2008.

[38] V. Ya. Zyryanov , V. A. Gunyakov , S. A. Myslivets , V. G. Arkhipkin, and V. F. Shabanov, Electrooptical Switching in a One-Dimensional Photonic Crystal, *Mol. Cryst. Liq. Cryst.*, 488, 118-126, 2008.

[39] A. Denisov and J. L. de Bougrenet de la Tocnaye, Photonic Crystals based on Cholesteric Liquid Crystals, *Mol. Cryst. Liq. Cryst.*, 494, 179-186, 2008.

[40] S. S. Choi, S. M. Morris, W. T. S. Huck, and H. J. Coles, Electrically Tuneable Liquid Crystal Photonic Bandgaps, *Adv. Mater.*, 21, 3915–3918, 2009.

[41] I. C. Khoo, A. Diaz, J. Liou, D. Werner, J. H. Park, Y. Ma, and J. Huang, Liquid Crystal Nonlinear Optical Meta-Materials, *Mol. Cryst. Liq. Cryst.*, 502, 109-120, 2009.

[42] J. Cos, J. Ferre-Borrull, J. Pallares, L.F. Marsal, Tunable Fabry–Pérot filter based on one-dimensional photonic crystals with liquid crystal components, *Opt. Commun*., 282, 1220-1225, 2009.

[43] H. L. Ong, Optically induced Freedericksz transition and bistability in a nematic liquid crystal, *Phys. Rev. A*, 28, 2393-2407, 1983.

[44] A. Taflove, *Computational electrodynamics: The Finite Difference Time Domain method*, Artech House, Boston, 2005.

[45] J. B. Pendry, and A. MacKinnon, Calculation of photon dispersion relations, *Phys. Rev. Letts.*, 69, 2772-2775, 1992.

[46] J. Jin, *The Finite Element Method in Electromagnetics*, John Wiley and Sons, New York, 2002.

[47] S. Obayya, M. F. O. Hameed, N. F. F. Areed, *Computational Liquid Crystal Photonics: Fundamentals, Modelling, and Applications*, John Wiley and Sons, United Kingdom, 2016.

[48] J. A. Kong, *Electromagnetic Wave Theory*, John Wiley & Sons, New York, 1986.

[49] P. Yeh, *Optics Waves in Layered Media*, John Wiley & Sons, New York, 1988.

[50] M. Born and E. Wolf, *Principle of Optics*, Pergmon Press, Oxford, 1999.

[51] M. S. Mohamed, M. F. O. Hameed, M. M. El-Okr, S. S. A. Obayya, Characterization of One Dimensional Liquid Crystal Photonic Crystal Structure, *Optik - International Journal for Light and Electron Optics*. http://dx.doi.org/10.1016/j.ijleo.2016.06.101

[52] J. Gosciniak, D. T. H. Tan, Theoretical investigation of graphene-based photonic modulators *Sci. Rep.* 3, 2013. doi:10.1038/srep01897

[53] Q. Zhu and Y. Zhang, Defect modes and wavelength tuning of one dimensional photonic crystal with lithium niobate, Optik, 120, 195–198, 2009.

[54] S. G. Moiseev, V. A. Ostatochnikovand D. I. Sementsov, Defect mode suppression in a photonic crystal structure with a resonance nanocomposite layer, *Quantum Electron.* 42, 557-560, 2012.

[55] S. G. Moiseev and V. Ostatochnikov, Influence of the Size-Dependent Permittivity of Metal Inclusions on the Optical Characteristics of a One-Dimensional Photonic Crystal with a Nanocomposite Defect, *Opti. Quant. Electr.*, 47, 3193-3200, 2015.

LIST OF PUBLICATIONS

Part of the thesis published and communicated in the refereed journals:

1. **Pawan Singh,** Narinder Kumar, Khem B. Thapa*, Devesh Kumar, Tunable transmission of a nematic liquid crystal defect in 1D periodic structure of dielectric materials due to orientation/re-orientation of nematic molecules, *in European Journal of Physics E (EPJ E)*, 41, 100, 2018.
2. **Pawan Singh,** Khem B Thapa, Narinder Kumar, Krishan Pal and Devesh Kumar, Graphene layers on semi-finite 1D asymmetric periodic structure of Si/Glass materials with defect of nematic liquid crystal for a sensor device, *Mater. Res. Express*, 6, 066209, 2019.
3. **Pawan Singh,** Khem B. Thapa, Narinder Kumar, Devendra Singh, Devesh Kumar, Study of transmission property of periodic layer consisting of SiO_2 and TiO_2 layers with anisotropic liquid crystal (LC) and $LiNbO_3$ as defect layers for optical switching, *Results in Physics*, 13, 102346, 2019.
4. **Pawan Singh,** Khem B. Thapa, Narinder Kumar, Devendra Singh, Devesh Kumar, Effective optical properties of one-dimensional periodic structure of TiO_2 and SiO_2 layers with a defect layer of nano-composite consisting of silver nanoparticle and E7 liquid crystal, *Pramana- Journal of Physics*, 93, 50, 2019.
5. **Pawan Singh,** Vivek K. Nautiyal, Ram Janma, Khem B. Thapa, Theoretical investigation of one-dimensional periodic structure of TiO_2/SiO_2 layers containing a defect layer of the nanocomposite with different radii of silver nanoparticles in the host liquid crystal, *Physica Scripta*, 95(6), 065507, 2020.
6. **Pawan Singh**, Khem B. Thapa, Narinder Kumar, Anil K. Yadav, Devesh Kumar, Tunable optical filter based on one-dimensional periodic structure composed of SiO_2 and anisotropic meta-material with a liquid crystal defect layer sandwiched by SiO_2, *International Journal of Modern Physics B*, 33, 950194, 2019.
7. **Pawan Singh,** Khem B. Thapa, And Girijesh N. Pandey, Temperature sensor and monochromatic filter based on one-dimensional photonic crystal containing Si and SiO_2 with a defect layer of liquid crystal, *Optoelectronics and Advanced Materials – Rapid Communications*, 13, 401, 2019.

8. **Pawan Singh,** Khem. B. Thapa, Narinder Kumar, and Devesh Kumar, Omnidirectional reflection band of one dimensional periodic structure (1DPS) of Si/SiO_2 with defect mode of nematic liquid crystal (5CB), *Journal of Physical Science*, 30(3), 117, 2019.
9. **Pawan Singh,** Krishan Pal, Khem B. Thapa, Narinder Kumar, Devesh Kumar, Embedded Liquid Crystal Defect with Graphene Layers in Asymmetric One-Dimensional Photonic Crystal as Sensor Application, Book Chapter in CRC Press, *Advances in Photonic Crystals and Devices,* 2019.
10. **Pawan Singh,** Krishan Pal, Narinder Kumar, Sudesh K. Singh, Khem B. Thapa, Devesh Kumar, Tunable Sensing Property of 1D Periodic Structure with Defect of Liquid Crystal Sandwiched by Metallic Layers, *Sensor Letters*, 17(10), 800, 2019.
11. **Pawan Singh,** Khem B. Thapa, & Sudesh K. Singh & Alok K. Gupta, Study of design tunable optical sensor and monochromatic filter of the one-dimensional periodic structure of TiO_2/MgF_2 with defect layer of liquid crystal (LC) sandwiched with two silver layers, *Plasmonics*, 2020.
12. Krishan Pal, **Pawan Singh,** Abhishikta Bhaduri, Khem B. Thapa, Current challenges and future prospects for a highly efficient (>20%) kesterite CZTS solar cell: A review, *Solar Energy Materials and Solar Cells*, 196, 138-156, 2019.
13. Narinder Kumar, **Pawan Singh,** Pranav Upadhyay, Shivani Chaudhary, Khem B Thapa, AK Dwivedi, Devesh Kumar, Odd–even effect of 7O. m liquid crystal compound series studied under the effect of the electric field by density functional theory (DFT) methods, *The European Physical Journal Plus (EPJ P)*, 135(5), 388, 2020.
14. Roshni Maurya, **Pawan Singh,** Prabal P. Singh, Krishan Pal, Girijesh N Pandey, Khem B. Thapa, Absorption and bandwidth properties of graphene based 1D-photonic crystal for THz devices, *AIP Conference Proceedings*, 2220(1), 020084, 2020.
15. Asish Kumar, **Pawan Singh,** Krishan Pal, Narendra Kumar, and Khem B. Thapa, Broadband reflector of 1D photonic crystal containing TiO_2/SiO_2 material at visible region, *AIP Conference Proceedings,* 2220, 020068 (2020).

16. Narinder Kumar, **Pawan Singh,** Khem B. Thapa, Devesh Kumar, Molecular spectroscopy and adverse optical properties of N-(p-hexyloxy-benzylidene)–p-toluidine (HBT) liquid crystal molecule studied by DFT methodology, *IOP SciNotes*, 1(1), 015202, 2020.
17. Narinder Kumar, **Pawan Singh,** Shivani Chaudhary, Khem B. Thapa, Pranav Upadhyay, Devesh Kumar, Spectroscopy Exiting behind the Electro-Optical Properties with an Even-Odd Effect of nCB Liquid Crystal Molecules: A Theoretical Approach, Acta Physica Polonica A, 137, 1135, 2020.
18. Asish Kumar, **Pawan Singh**, Khem B. Thapa, Study of super absorption properties of 1D graphene and dielectric photonic crystal for novel applications, *Opt. Quan. Electronics*, 52, 1, 2020.
19. Narinder Kumar, Shivani Chaudhary, **Pawan Singh,** Khem B. Thapa, Devesh Kumar, Electro-optical odd-even effect of APAPA liquid crystal molecules studied under the influence of an extraneous electric field (THz): A theoretical approach, *J. Mol. Liq.,* 318, 114254, 2020.
20. Narinder Kumar, **Pawan Singh**, Khem B. Thapa, and Devesh Kumar, Electro-optical effect of the nCOOCB liquid crystal molecules under the terahertz (THz) frequency range: A theoretical approach, *Journal of Physical Science (Accepted)*, 2020.
21. Narinder Kumar, **Pawan Singh**, Khem B. Thapa, and Devesh Kumar Odd-Even effect observed in the electro-optical properties of the homologous series of HnCBP liquid crystal studied under the impact of the electric field: A theoretical approach, *Iranian Journal of Mathematical Chemistry (Accepted)*, 2020.