ABSTRACT

Liquid crystals (LCs) exhibit a unique combination of fluidity and long-range molecular order. This gives rise to anisotropic optical, dielectric, and electro-optic properties that are widely exploited in displays, photonic devices, and sensing technologies. However, the inherent physical properties of conventional LCs often limit their performance in applications requiring faster electro-optic response, higher photoluminescence, enhanced optical modulation, higher environmental stability, and sensitive chemical detection. A powerful strategy to overcome these limitations is their integration with the functional organic and inorganic dopants, which can enable precise modulation of their dielectric, electro-optic, ionic, photophysical, chiro-optic, and sensing properties. This thesis focuses on the systematic design and development of functional LC composites through the incorporation of ferroelectric nanoparticles (NPs), conjugated polymer NPs, aggregation-induced emission (AIE) active chiral dopants, pseudopeptide gelators, and protonatable chiral molecules, aiming to realize tunable electro-optic, photoluminescent, smart window, and gas-sensing devices.

The first objective of this work is to investigate the influence of ferroelectric $BaTiO_3$ nanoparticles (NPs) of two different size ranges (5-15 nm and 50-70 nm) on the dielectric, electro-optic, and ionic properties of an antiferroelectric bent-core LC. The incorporation of $BaTiO_3$ NPs lowers the phase transition temperatures and modifies the dielectric relaxation behavior of the antiferroelectric SmA phase. The spontaneous polarization decreases from 71 nC/cm^2 for the pure LC to 48 nC/cm^2 and 61 nC/cm^2 for the smaller NPs (5-15 nm) doped LC and larger NPs (50-70 nm) doped LC, respectively, indicating antiparallel dipole-dipole correlations between the ferroelectric NPs and LC molecules. A reduction in response time of approximately 7.1% for the smaller-sized NPs (5-15 nm) doped LC and 30.7% for the larger-sized NPs (50-70 nm) doped LC demonstrates enhanced electro-optic switching performance. Furthermore, direct current conductivity increases by nearly 3.2-fold and 1.6-fold for the smaller (5-15 nm) and higher size (50-70 nm) NPs doped LC, respectively. The smaller-sized NPs (5-15 nm) additionally reduce ionic contamination by about 16%, suggesting their ion-capturing capability. These findings reveal that both NPs' size and ferroelectricity strongly influence the electro-optic and ion-transport properties of bent-core LC nanocomposites, making them promising candidates for fast-switching electro-optic applications.

The second objective explores the role of conjugated polymer nanoparticles (PNPs) based on poly(3-hexylthiophene) (P3HT) derivatives in tuning the ionic properties of nematic LC and

stabilizing blue-phase LC (BPLC). PNPs with an average size of 15.5 nm, incorporated at concentrations of 0.01 and 0.1 wt.% in 5CB LC, significantly enhance the ionic transport properties. Nearly two orders of magnitude increase in direct current conductivity and ion diffusion coefficient, while the mobile ion concentration increases by only ~1.5-fold. These results indicate enhanced ion transport in the nematic host due to the intrinsically conducting nature of the polymer NPs. Furthermore, incorporation of smaller-sized PNPs (~5 nm) into BPLC at optimized concentrations of 0.005 and 0.01 wt.% gives a phase stabilization effect, with a maximum BP range enhancement of ~3 °C observed for the 0.005 wt.% concentration. The electro-optic performance is markedly improved, with hysteresis reduced from 70% to 0.1% and residual birefringence decreased from 2.9% to 0.1%. In addition, at 0.01 wt.% concentration of PNPs, nearly 70% enhancement in photoluminescence intensity is observed. These findings demonstrate that conjugated polymer NPs effectively improve ionic transport, thermal stability, electro-optic response, and luminescence characteristics of LC systems, highlighting their potential for advanced photonic and display applications.

Objective three focuses on the development of tunable luminescent LC systems through the incorporation of a pseudopeptide-based aggregation-induced emission (AIE)-active chiral dopant into nematic and smectic-A LC hosts. Polarized optical microscopy and circular dichroism spectroscopy confirm efficient chirality transfer and the formation of a helical cholesteric (N*) phase, whereas the induced smectic-A* phase does not exhibit helical organization. Temperature-dependent photoluminescence studies reveal a strong influence of LC ordering on the AIE characteristics. Circularly polarized luminescence (CPL) is observed in the N* phase, where supramolecular helical ordering and AIE coexist, yielding a maximum luminescence dissymmetry factor (g_{lum}) of 0.071 in the doped 5CB LC. In comparison, the self-assembled chiral aggregate of the dopant in 90% H_2O/DMSO exhibits comparatively lower g_{lum}value of -0.0025, highlighting the role of the LC helical environment in amplifying CPL. The electrically switchable N* LC displays distinct states with haze values of 45%, 4%, and 2% for planar, focal-conic, and homeotropic states, respectively, demonstrating efficient voltage-controlled light modulation for smart-window applications. Furthermore, nearly threefold enhancement in photoluminescence intensity is observed in the focal-conic state, while the induced SmA* phase exhibits approximately 80% higher photoluminescence intensity compared to the N* phase in the doped LC. These multifunctional LC composites therefore provide an effective platform for CPL, electrically tunable smart windows, and luminescent photonic devices.

Objective four demonstrates the development of nematic and N* LC physical gels using a pseudopeptide-based gelator capable of forming fibrous supramolecular assemblies for smart-window applications. The gel morphology, viscoelastic response, and electro-optic properties are found to be strongly dependent on gelator concentration and LC phase. Four different gelator concentrations (1, 2, 3, and 4 wt.%) are investigated in nematic 5CB, while a 2 wt.% gelator concentration is optimized for the N* LC system. Among the nematic gels, the 3 wt. % composition exhibits optimized electro-optic performance in a window device with a contrast ratio of 49.01, threshold electric field of 0.64 V/µm, operating electric field of 4.21 V/µm, rise time of 51.8 ms, and fall time of 55.4 ms. In comparison, the N* gel containing 2 wt.% gelator shows a higher contrast ratio of 167, along with a threshold electric field of 1.50 V/µm, operating electric field of 4.64 V/µm, rise time of 67 ms, and fall time of 91 ms. The superior contrast ratio observed in the N* gel highlights the advantage of light-scattering focal conic state entangled in gel networks for smart-window applications, whereas the nematic gel demonstrates comparatively faster electro-optic switching. These results establish pseudopeptide-based LC gels as promising candidates for electrically switchable smart windows.

Objective five reports the design and development of an N* LC-based optical sensor using a strategically designed chiral dopant bearing a protonatable moiety for selective detection of hydrochloric acid (HCl) fumes. Protonation of the chiral dopant upon exposure to HCl leads to a change in helical twisting power, resulting in a measurable shift in the selective reflection wavelength of the N* LC. The sensor exhibits a detection of HCl vapors in the parts-per-million (ppm) range, with a sensitivity of approximately 3.26 nm ppm^{-1}.

The thesis concludes with an outlook on the future scope of the developed NP-LC composites, AIE-active and sensing chiral LC systems, and supramolecular LC gels, highlighting their potential for advanced electro-optic and photonic applications, including electrically tunable smart windows, luminescent displays, adaptive light-scattering and diffusion devices, and smart sensors.