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## Chapter

# Overview of Liquid Crystal Research: Computational Advancements, Challenges, Future Prospects and Applications

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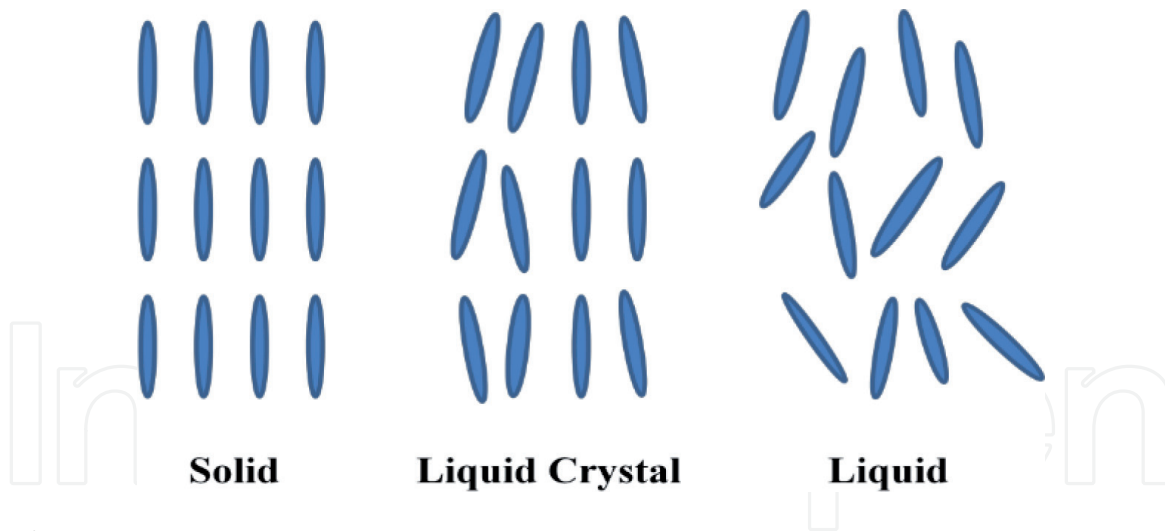
## Abstract

Liquid crystal (LC) is a fascinating state of matter that combines order and mobility at multiple hierarchical levels, spanning from nanoscale to the macroscale, or from molecular to the macroscopic, and is composed of molecules and layers as thin as of a few nanometer in size. This unique combination allows such a system to adapt to a wide range of external stimuli, including temperature, magnetic field, electric field, mechanical stress, light, chemical reaction, and electrochemical response, by determining a new lowest energy configuration. Liquid crystalline nanostructures efficiently transmit and amplify information and attributes over macroscopic sizes due to their dynamic nature. The responsiveness and diversity of LCs provide enormous potential and challenges for fundamental scientific insights as well as opening the door to countless applied applications. Recent breakthroughs in nanotechnology have boosted the discipline, both in terms of theoretical simulations and the ability to fabricate nanoscale structures such as sub-wavelength gratings, nanoporous materials, and nanoparticles. Because LC materials are switchable, a new family of active plasmonic and nanophotonic devices is emerging, describing fascinating basic research processes as well as the creation of upgraded devices. This chapter discusses the fundamentals, computational advances, future prospects and challenges, as well as potential applications of LCs.

**Keywords:** liquid crystals, fundamentals, future prospects and challenges, computational advances

## 1. Introduction

Liquid crystals investigation was begun by an Austrian scientist, Friedrich Reinitzer in 1888 when he espied a material named cholesteryl benzoate having two different melting points. He manipulated the temperature of the samples in his experiments and observed the changes that happened. Due to this early work, Reinitzer is attributed with the discovery of a new phase of matter - the liquid crystal phase and since then, liquid crystals have been under study for various



**Figure 1.**  
*A comparison of solid, liquid and liquid crystal orientation [7].*

research fields including physics, chemistry, medicine as well as engineering that resulted in the advanced nanostructured liquid crystals exhibiting an extraordinary ordered pattern and highlighting advanced functions such as electro-optical effects, chromism, sensing and templating [1–3].

The state of matter which shows liquid and crystalline properties at the same time is known as a liquid crystal, and this dual state of matter not only possesses viscous properties like fluidity, formation of droplets and mechanical properties but also exhibits the nature of crystalline solids such as periodic and anisotropic properties; therefore, they are named mesophases [4]. Liquid crystals are gaining popularity due to their remarkable functional properties, due to their ability to respond to external stimuli such as heat, light, electric fields, and mechanical forces [5]. Liquid phase molecules have no defined intrinsic order, while solid molecules are highly ordered, and the distinguishing property of liquid crystal is the inclination of molecules to point along the same direction of axis, called an anisotropic property [6] as shown in **Figure 1** [7]. Liquid crystals are classified into two primary groups based on various conditions and parameters: thermotropic and lyotropic liquid crystals, which differ in their arrangement mechanism but share many properties.

Thermotropic liquid crystals may be created by heating crystalline structures, which causes molecular position order to disappear but not the molecular orientational order, resulting in a dynamic phase with anisotropic liquid crystal characteristics [8]. This type of liquid crystal is temperature-dependent, with high temperatures resulting in an ordinary isotropic liquid phase owing to disrupted phase ordering, and low temperatures resulting in an anisotropic ordered crystalline liquid phase. On the other hand, an organized structure in a colloidal solution creates lyotropic liquid crystals that are formed by amphiphilic molecules with hydrophilic and hydrophobic portions. By changing the concentration and temperature of amphiphilic molecules, different lyotropic phases may be produced [9].

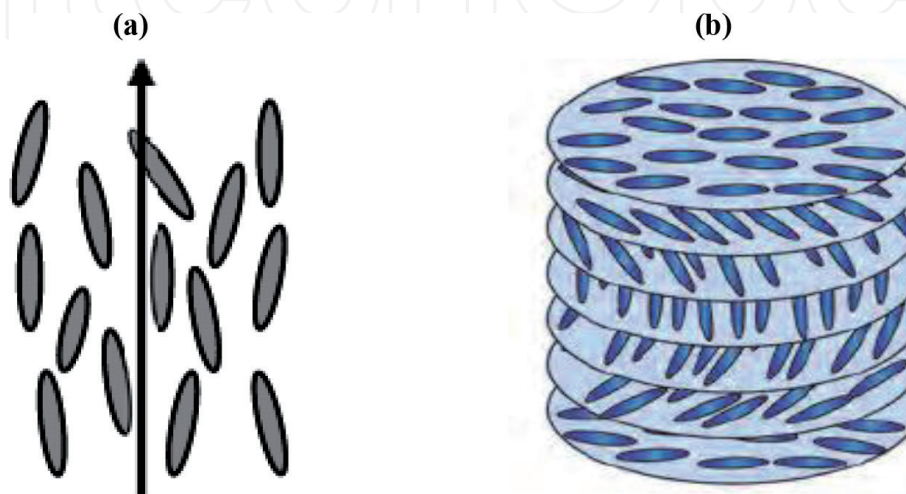
## 2. Fundamentals of liquid crystals

Liquid crystal classifications on an extensive level open up ways for various fundamental meso-phases. The chemical and physical properties of liquid crystals vary by changing temperature, solution concentration and other parameters that resulted in long-range orientational as well as positional order of molecules.

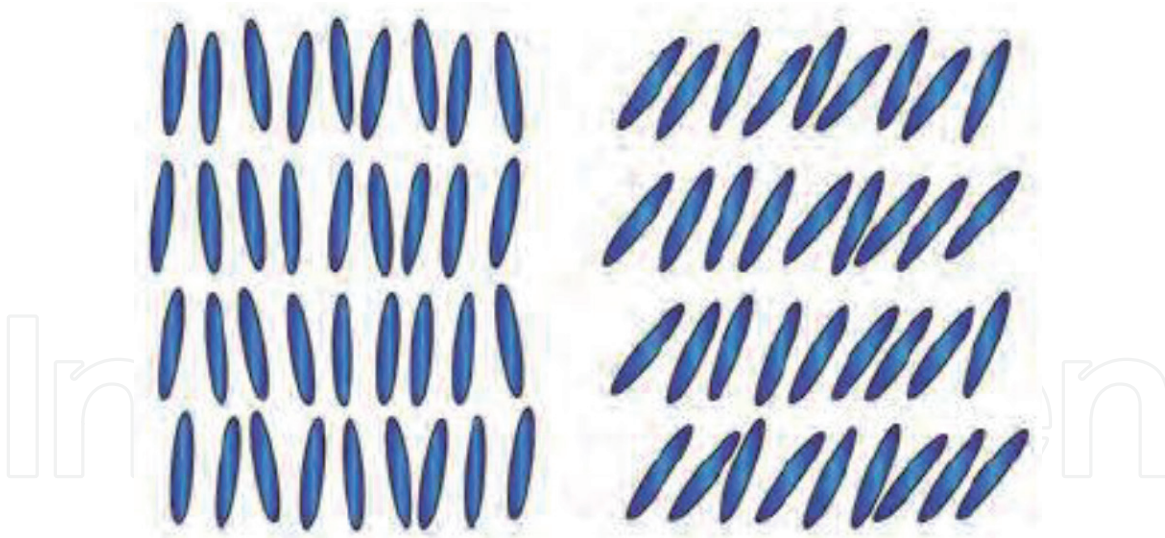
Thermotropic liquid crystals result in different kinds of meso-phases due to varying temperatures, and these transitions are controlled thermally. The mechanism further divides thermotropic liquid crystals into two categories: enantiotropic liquid crystals, which can be obtained by only decreasing the liquid temperature or increasing the solid temperature, and monotropic liquid crystals, which can be obtained by either increasing the temperature of a solid-state material or decreasing the temperature of a liquid state material to form an aligned as well as ordered liquid crystal arrangement. Depending on the molecular arrangement and symmetry, thermotropic liquid crystals are subdivided into four main categories; nematics, cholesterics, smectics, and columnar liquid crystals. The orientational order, positional order, and bond orientational order are some of the characteristics that describe liquid crystal formations. Nematic mesophase is the fundamental liquid crystal phase in which the molecular orientation is correlated with local molecular-axis orientation that can be controlled by external factors like; an electric field that helps the molecular axis to align accordingly [10], as is shown in **Figure 2(a)** [11]. These liquid crystal structures have a long-range orientational order but they lack in order of molecular center of mass positions, and are anisotropic having a rigid molecular backbone that outlines the long axis of molecules. Because they have a strong dipole moment and a high refractive index, these crystalline compounds may easily be polarized, making them useful in display applications [12].

Cholesteric liquid crystal state is comparable to nematic state [13], having nematic layers where each layer has its director; therefore, it is known as the counterpart of the nematic phase, as is shown in **Figure 2(b)** [14]. Likewise, these compounds exhibit long-range orientational order owing to their molecular organization into a long axis that is parallel to the molecular plan, and the molecular axis is defined as helical. The cholesteric structure is characterized by the pitch that is the distance along the long-axis on which the director rotates. Cholesterics are finite pitch structures with a few hundred nanometers of pitch; however, nematics can also be of the finite pitch if doped with an enantiomorphic compound. Cholesteric structure pitch is comparable to visible light, resulting in white light scattering owing to Bragg's reflection phenomenon, which may be exploited for different optical applications although this pitch can also be sensitive to numerous variables [15–17].

Smectic liquid crystals differ from others owing to layer ordering but molecule orientation is comparable to nematic in addition to layer alignment, and these structures have both positional and orientational orders. The smectic liquid crystal phases exhibit molecules organized perpendicular to layers, hexagonally structured,



**Figure 2.**  
(a) Nematic liquid crystal [11], (b) cholesteric liquid crystal schematic diagram [14].

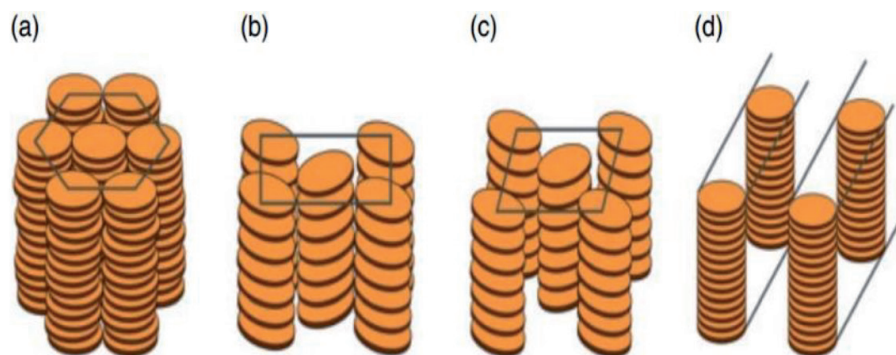


**Figure 3.** Smectic A, Smectic C liquid crystal schematic diagram [12].

and tilt angle measurement in smectic types A, B, and C; however, they are more ordered than the nematic liquid crystal phases. **Figure 3** depicts smectic A and C with no molecular positional order inside each individual layer, where smectic A molecules are orientated perpendicular along with the layer, but smectic C molecules are tilted away from the layer orientation, and so have order in one direction only.

Columnar liquid crystals are also known as discotic liquid crystals due to the disc-shaped molecular structures that are stacked in column form and organized in various shapes [18], while the columnar phase molecules are classified based on their packing motivations. They are arranged in 2D patterns such as hexagonal, rectangular, oblique, and lamellar [19] and these molecules are stacked in their respective lattices as shown in **Figure 4**.

Another classification of liquid crystal, lyotropic liquid crystal transitions, occurred by changing solvent concentration as well as varying the temperature. Amphiphilic molecules in a solution with hydrophobic and hydrophilic components resulted in diverse lyotropic liquid crystals and varied concentrations resulted in various circular or rod-shaped micelles in a solution. The rod-shaped micelles are arranged to form highly viscous hexagonal lyotropic liquid crystal while the circular micelle form a cubic pattern of lyotropic liquid crystal that does not have shear planes to make them more viscous than the hexagonal lyotropic phase.



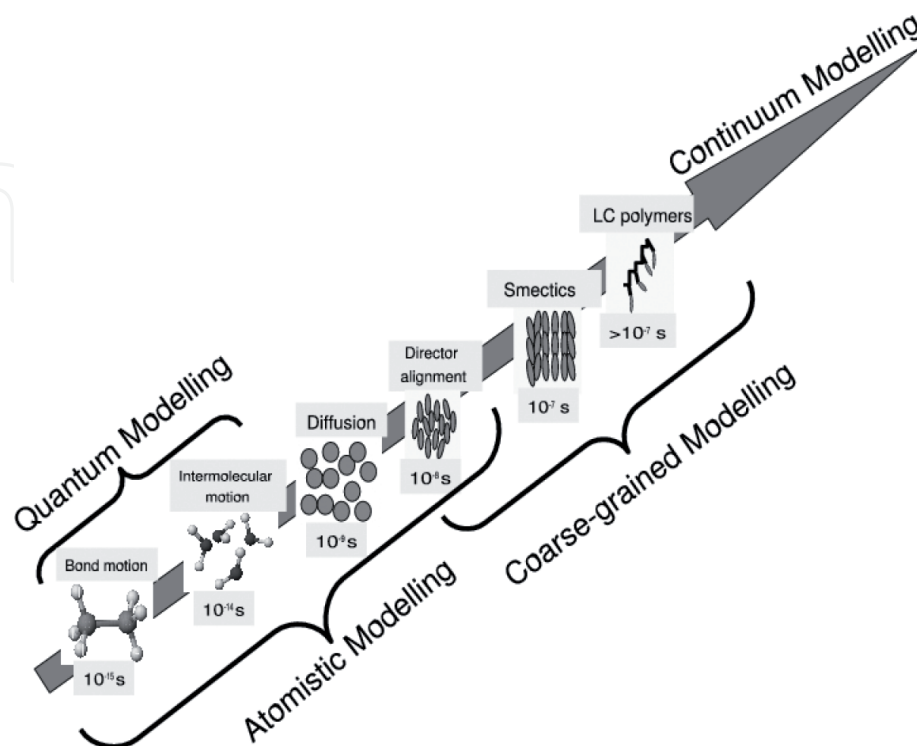
**Figure 4.** Columnar phase liquid crystals schematic diagram; (a) hexagonal, (b) rectangle, (c) oblique, and (d) lamellar [19].

Shape-dependent numerous kinds of lyotropic liquid crystals can be obtained by manipulating the micelle shape present in the solution [20, 21].

### 3. Computational advancements

There have been relatively few computational approaches to the advancement of liquid crystals since their discovery. In the 1940s, Onsager showed the colloidal solution method for liquid crystal formation, and proved that transitions can be occurred from isotropic to anisotropic phase by changing the density [22]. Then, in the 1950s, Maier and Saupe developed the molecular mean-field theory that explained the temperature-dependent transitions of thermotropic liquid crystals [23]; however, in comparison to these theories, the first simulation theory linked to simple liquid crystals was developed in the 1990s [24]. In recent years, attempts have been made to investigate simulation approaches and methodologies for determining the functions and properties of liquid crystals. The most challenging aspect in molecular simulation is connecting different lengths as well as the time of action scales, and various models are employed to manage these simulations based on their time scales, as shown in **Figure 5**. Molecular bonds and intermolecular motions in the femto-second time scale range are addressed by quantum modeling, while atomistic modeling handles molecular bond motion to liquid crystal director alignment in the femto-to-nanosecond time scale. The coarse-grained approach facilitated simulations of liquid crystal polymers at nanosecond to microsecond time scales, whereas continuum modeling is better suited to simulations at longer length and time scales.

Quantum modeling mainly addressed the intermolecular motion with a time scale range of femto-seconds, whereas atomistic modeling is considered to be the vanguard of computational analysis of nanomaterials, and it plays a pivotal role as an interfacial region. The building complex models have also proven to be an effective tool for predicting the relationship between macroscopic properties and



**Figure 5.**  
*Computational schemes employed in liquid crystals research [25].*

underlying atomistic structures. The structural analysis of a material is obtained at the end of molecular dynamics or Monte Carlo simulations, and it reflects the pair correlation function, which yields the probability of atomic separation by some calculated distance, and it can then be compared with experimental data to validate the computational as well as model methodology, ensuring that results correspond to the experimental setup. The coarse-grained models are vital for the illustration of complex systems that allow keeping the main entities and performing the important simulations that are not more suitable with other simulation methods like molecular dynamics having some limitations in time and length scales. The group of atoms is bounded by beads whose interaction depends on their internal energy function which accounts for the detailed simulations at the atomistic level for both bonded and non-bonded interactions. This modelling method can be applied to a wide range of length scales, such as a bead or interaction site of a group of atoms, a functional group, or a polymeric micro-particle, depending entirely on the system of interest and the investigated property [26].

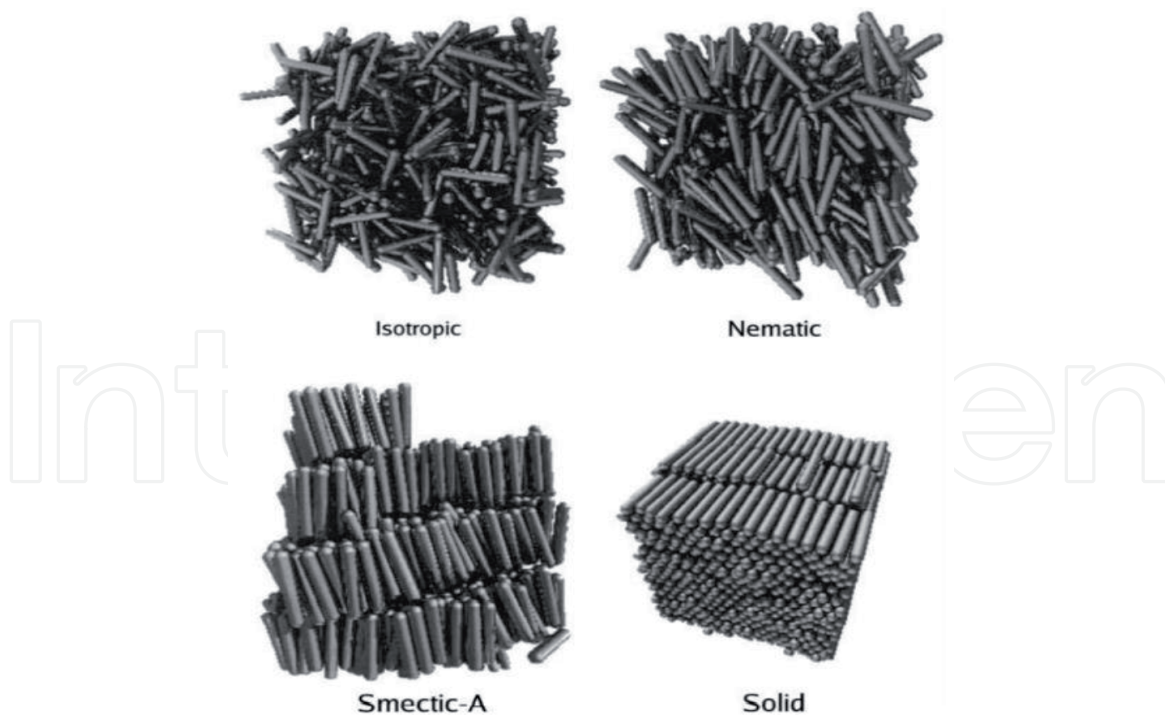
Continuum models are proved as the most useful description of lateral composition segregation that measures the tendency of a solid solution to possess the phase separation. It has also been reported that continuum simulation is more feasible for more precise modeling of the mechanics problem of stress relaxation by lateral region formation of phase-separated material, where the system goes from constrained to less-stressed configuration and the tendency towards phase separation may decrease. The kinetics of morphological evolution reflects these transitions and is a superior alternative for simulations with larger lengths and time scales [27]. Molecular modeling becomes difficult as the length and time scales increase, thus various sophisticated simulation techniques are employed, including lattice Boltzmann nematic-dynamics [28], reduction of the Landau-de Gennes free energy [29], and continuum theory approaches [30]. The liquid crystal force field method is appropriate for a wide range of molecular stands. Bond stretching, bond bending, and torsional potential may be calculated using ab-initio / DFT [31] calculations and the force field approach in combination with sophisticated computer technology.

### 3.1 Recent classifications of liquid crystals

The recent advancements in computer simulation of liquid crystals classified them into three main categories; hard non-spherical models, soft non-spherical models and lattice models.

#### 3.1.1 Hard non-spherical model

The hard non-spherical model is based on the fact that liquid crystal molecules are generally non-spherical hard ellipsoids, and hard sphero-cylinders, as shown in **Figure 6**. This intriguing feature would be useful in studying the basic effects and assessing the liquid crystal stability as well as other external stimuli interactions, whereas the phase behavior of these hard molecule-based models is reliant on density changes and is independent of temperature. This feature of liquid crystal molecules is demonstrated by Onsager's work [22], in which he deduced that transitions from isotropic to anisotropic occur well below the density at which the system would be expected to crystallize, provided that length is much greater than the diameter, and represent a non-spherical pattern. The interplay between translational and rotational entropy is the driving factor behind liquid crystal formation; as density increases the system minimizes its free energy by organizing itself, causing a rise in translational and rotational entropy.



**Figure 6.**  
*Simulations of hard spherocylinders with aspect ratio  $L/D = 5$  at different densities [32].*

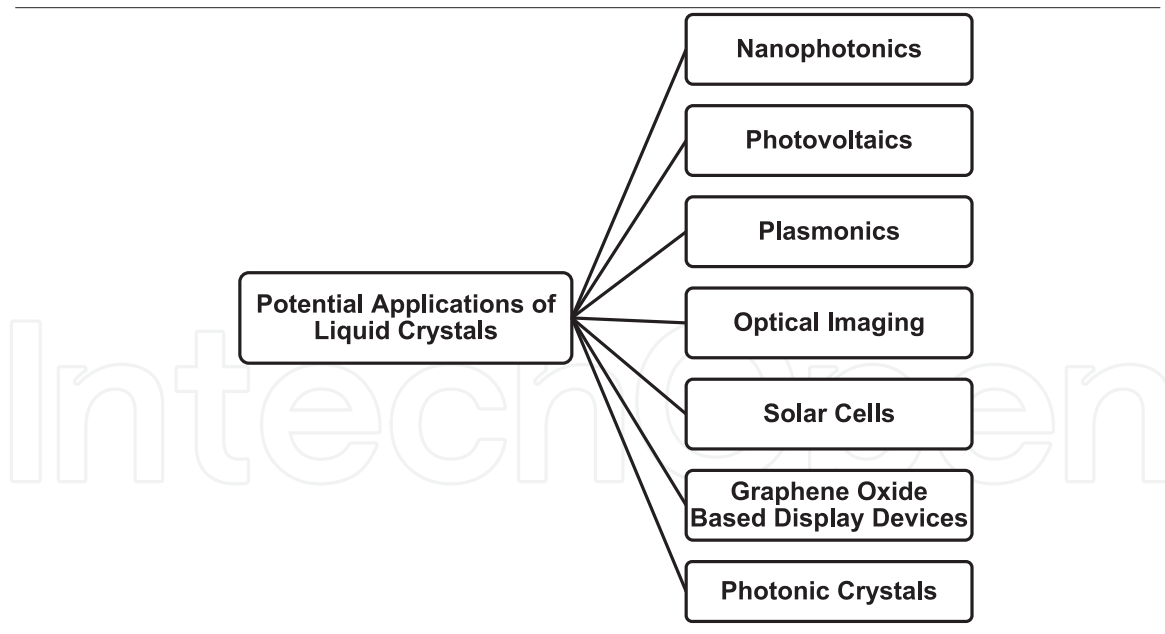
### 3.1.2 Soft non-spherical model

Non-spherical simulations were done in the 1970s and subsequent years, but due to a lack of computer time, these simulations were not completed properly [33–35]. The original work has recently been expanded by combining thermodynamic and dynamical characteristics to calculate the value of electrons for non-spherical (ellipsoids) molecules and adding boundary constraints to decrease surface effects [36], revealing spontaneous liquid crystal ordering by an even compression of the isotropic state beyond the thermodynamic stable limit. However, using the molecular dynamic approach, it was discovered that the smectic phase develops from the nematic phase over time. This method allows for the comparison of diffusion coefficients parallel to smectic planes, which reveals mobility within layers and motion between layers in the perpendicular direction.

Liquid crystal molecules in a soft non-spherical model are soft and feature long-range molecular interactions, whereas temperature is used to determine thermodynamic equilibrium in this model, which was not studied in hard non-spherical models. The invention of the Gaussian overlap model [37] started work in this field in the 1970s, and the Gay-Berne potential is the most often used soft non-spherical model. This model, which was founded on the notion of fitting the potentials to a more exact atomic model of the molecule of interest [38], incorporates the attraction of soft ellipsoids, which have the same symmetry as hard ellipsoids. Although, the initial potential had unrealistic features, it has subsequently been improved and widely used [36]. The Gay-Berne (GB) model has the advantage of being able to explore a wide range of interactions between various thermotropic liquid crystals by adjusting the potential and well-depth parameters, as well as being simple to combine with other potentials. Recent results combine GB and a point dipole to illustrate the ferroelectric phase [39], as well as GB with a point quadrupole to demonstrate the smectic C phase [40]. Because this model includes a temperature factor, an isotropic phase was formed at high temperatures, but upon cooling, a nematic phase was observed, indicating that the smectic A phase was obtained, while further cooling yielded hexagonal alignment within the layers, indicating that the smectic







**Table 1.**  
*Potential application domains of liquid crystal research.*

#### 4.1 Graphene oxide liquid crystals

Graphene is an atomic-scale thin carbon material that has drawn much attention due to its unique and extraordinary electrical, chemical, thermal, mechanical and optoelectronic properties having a wide range of applications. Chemical oxidation of graphene produces graphene oxide, while wet chemical exfoliation of graphene produces graphene oxide-based liquid crystals [44]. Graphene oxide is unique in comparison to liquid crystal molecules because of its large diameter to thickness aspect ratio and optical anisotropy, exhibiting a strong magnetic response. Graphene oxide-based liquid crystals are employed in many display and device applications due to their electric field-induced birefringence. The devices based on graphene oxide consume less power than traditional liquid crystals and do not require specific electrode treatment. Also, the device size and switching time may be reduced by decreasing the size of the graphene oxide flakes [45]. When the size of the graphene oxide flakes decreases, the polarization anisotropy reduces quicker than the rotational viscosity, causing the rising time to increase, while falling time is controlled only by rotational viscosity, smaller flakes suffer less, resulting in a decrease in falling time, although, the smaller switching time is required for screen applications. Graphene oxide liquid crystals may also be utilized as rewritable boards with a dark or bright background [46], a reflective display that does not require polarizing optics and relies only on ambient light. These reflective displays which are controlled by an electric field are extensively used in electronic books because of their low energy consumption and inexpensive cost.

#### 4.2 Photonic crystals

Liquid crystals have remarkable optical properties that respond to external stimuli such as light, temperature, electric field, magnetic field, and electrochemical reactions resulting in a dynamic change of material from the molecular to the macroscopic level, and this dynamic system makes them more useful in the nanofabrication of photonic materials. The responses of liquid crystals to various stimuli contribute to the photo bandgap tuneability, which has several uses in

communication systems and optical integrated circuits. Photonic crystals can control photons and hence offer a wide variety of uses based on defect engineering or the crystal bandgap; consequently, light can only be transmitted by adding defects, while the simultaneous introduction of point and line defects produces a miniature photonic circuit for different applications [47–49]. Photonic crystals may also influence light propagation through the structure resulting in a change in the propagation direction, slower propagation speed, and negative refraction. Controlled photonic devices are potential instruments for optical switching, routing, optical imaging, and power splitting because of their capabilities. This approach may also be employed to develop lasers with a narrow wavelength range on a tiny chip [50]. It is worth noting that, owing to better photonic crystal fabrication, 3D photonic crystals, rather than the currently utilized 2D crystals, will be used in future applications due to greater light control in the 3D range. Photonic crystal fibers can transmit a large range of light wavelengths with zero dispersion, and due to this uncommon property, they can be widely used for communication networks, polarization splitters, rotators, filters as well as multiplexers [43].

### **4.3 Photovoltaics**

Liquid crystals are widely used in many photovoltaic devices owing to their unique intermolecular interactions. Discotic or columnar liquid crystals are more efficient to use and have more intermolecular interactions than inter-columnar interactions with special arrangements, in which each column acts as a molecular wire so that electrons and holes can move freely in one-dimensional structural arrangement and this alignment of molecules increases the electrical conductivity that allows them to be used in photovoltaic devices [51, 52]. Also, p-type and n-type discotic liquid crystals can be designed, and their properties, as well as alignment to the electrode surface, can be improved to achieve better charge migration results [53]. Calamitic or rod-like liquid crystals are also fascinating for semiconductor applications, particularly in display devices as well as conducting impurities [54]. In addition, liquid crystals create nanomorphology between the donor and acceptor layers to enhance film orientational order, resulting in efficient photocurrent generation and higher incoming photon conversion efficiency.

### **4.4 Nanophotonics**

A newly emerging field that combines liquid crystals with nano-sized photonic structures is called nanophotonics [55], and is widely used in numerous applications. These devices are utilized to tune plasmonic nanostructures, as well as nanoporous materials, controlled magnetic field for switching liquid crystals and these liquid crystal composites with dielectric nanostructures are continuously gaining practical attention [56]. Liquid crystals are enabling to impart their long-ranged orientational symmetry to nanomaterials. Low concentrations of nanomaterials can be oriented as nematic patterns that can demonstrate improved physical properties of liquid crystals as well as a strong response to external stimuli such as electro-optic and magneto-optic responses, electrochemical memory effect, and changes in liquid crystal orientational order parameters [57]. Furthermore, the ability of liquid crystals to flow and fill nano-gaps led to the development of adjustable photonic crystal devices, porous silicon thermal tuning, and 2D photonic bandgap structures filled with liquid crystals [58]. Because nematic liquid crystals have poor magnetic anisotropy, switching the device requires a high magnetic field of about one Tesla, which would damage the device, so combining liquid crystals with ferromagnetic nanoparticles can be used to improve device switching at low magnetic fields for

even better practical applications [59] that would result in some intriguing effects like increased dielectric anisotropy, increased order parameter as manifested by an increase in birefringence, enhanced non-linear effects, and so on, and these factors resulted in a decrease in threshold voltage, which is an important factor of power consumption in display applications [60].

#### 4.5 Plasmonics

Liquid crystals have gained much attention for plasmonic applications because of their attractive features such as; large birefringence, less driving threshold and various possible fabrication methods. This particular application of liquid crystals opens up the opportunities for next-generation plasmonic devices by combining both the liquid crystals and nanostructures with enhanced plasmonic properties resulted in devices such as; modulators, absorbers, plasmonic waveguides, plasmonic switches and color filters, etc. The main feature of liquid crystals that makes them suitable for active plasmonic devices is the difference in refractive index resulting in large birefringence. There are numerous ways to apply liquid crystals to the plasmonic nanostructures to get a promising change in refractive index that is essential for its potential device applications. Liquid crystal-based active plasmonic devices can be categorized according to the driving methods such as; electric field-driven method, heat-driven method, acoustic waves driven method and light-driven method. Depending on whether external biasing is supplied, such as an electric field, heat, light, or acoustic waves, liquid crystal molecules will align properly when exposed to external stimuli. This feature of liquid crystals is coupled with a periodic nanostructured material to produce the consequent controlled effect of plasmonic structures such as reflection, transmission, or absorption, indicating its potential in a variety of plasmonic-based devices [61]. Hence the combination of liquid crystals and metallic nanoparticles can be utilized to create tunable plasmonic devices, because metallic nanoparticles exhibit strong attenuation at resonance wavelengths that correspond to localized surface plasmon and this resonance wavelength can be modified by varying surrounding refractive index which can be controlled by external electric field using liquid crystals, yielding promising results [62, 63].

### 5. Current challenges and problems

Since the previous decade, liquid crystals have been a popular issue, with considerable progress made in understanding their complicated process and alignments in many applications, particularly in display devices, which makes them fascinating. However, quite some important alignment aspects are not understood well specifically regarding liquid crystals molecular interactions, which is the biggest challenge in the liquid crystals industry of this era. There is a need for the developed alignment technology that would resolve the existing limiting factors that are affecting display quality and processing costs. The specific challenging areas of liquid crystals include non-uniform alignment over large displays, image sticking, uneven display brightness and multi-domain alignment pattern configurations [64]. Response time of liquid crystals is another challenge that plays an important role in display applications. Slow response time of liquid crystal causes blur quality and undesirable image display which is due to the non-adjustable pre-tilt angle of liquid crystals with the substrate that eventually affects the cell dynamics. To improve image quality and display, a proper oriented angle adjustment between liquid crystals and substrate is needed to be addressed [65]. Furthermore, anchoring energy, which is the energy necessary to deviate the director off the molecular axis at a specific angle, may be

used to evaluate the alignment strength of the liquid crystal. Associated with the pre-tilt angle, stability of anchoring energy is another biggest challenge of liquid crystals industry to obtain uniform planer alignment, and to overcome this problem, rubbing mechanism was introduced to align liquid crystals, but this mechanism also faces challenges including static charge accumulation as well as dust-particle generation on crystal surface which affects the basic device characteristics and operational mechanism. The image sticking phenomena that happens when an image is shown for a long time is an essential aspect in determining the liquid crystal display quality. The present state of the problem of the liquid crystal [64] is indeed the electric charge or residual DC charge produced on the liquid crystal surface during long-term picture display, which causes selective surface adsorption of ionic impurities present in liquid crystal material or layers. Moreover, liquid crystals have some other drawbacks related to a huge number of ionic impurities present in aligned layers of liquid crystals and the presence of conjugated functional groups or lone pairs in liquid crystal molecules and between its aligned layers that would eventually result in disturbing as well as disrupting the display application, hence affecting the role of liquid crystals in device applications [66].

## **6. Future prospects**

Liquid crystals are materials with extraordinary properties mainly because of the partial orientational order having application in electronic, display and non-display devices that have become a pervasive as well as unavoidable feature in routine life. The full exploration of these materials is still a challenge due to the tricky problems involved in its phase structures, and a wide range of thermotropic liquid crystals with different shapes are reported with molecular self-assembly and interactions. Despite molecular shape and properties, fascinating research trends highlights the lack of systematic studies. However, this gap can be considered for future research by developing standard techniques and procedures. In addition, the molecules can be modified by the functional units to obtain highly functional systems using a variety of unexplored solutions.

The progression in nanophotonics can be used in combination with liquid crystals to design tunable devices with the help of powerful computer simulations which would continue assisting the building and understanding of liquid crystal devices at atomistic as well as a molecular level. Because of developing nano-sized liquid crystals, the future decade is likely to reveal more novel adjustable technologies, and this area needs strong developments to generate models as well as techniques with enhanced phase behavior representation diagrams which would lead to study the structural changes along-with phase behavior to explore novel material properties. Polyphilic molecules, which provide various interaction regions in a molecule to incorporate other flexible materials, are another intriguing feature of liquid crystals, and they can be more beneficial by controlling the molecular self-assembly, which is the most difficult part of synthetic engineering. However, if simulations are sophisticated enough to be utilized as engineering tool to create polyphilic liquid crystals with the desired structures; the liquid crystal industry can achieve amazing success.

## **7. Concluding remarks and summary**

This chapter summarized an overview of liquid crystals by exploring fundamentals along with its recent computational advancement, challenges faced, applied applications and future prospects. Liquid crystals are unique in their properties

having potential for numerous applied applications ranging from optical imaging, plasmonics, solar cells, photonic crystals, photovoltaics as well as nanophotonics, and the research in this field is the spark for the next forefront of economic development. Because of the combination of LCs with nanotechnology, the next decade will see noticeable developments and an increase in miniaturized tunable devices such as; tunable optical filters based on LCs and plasmonic phenomena like enhanced optical transmission through nano-slits, extinction of metallic nanoparticles and nanostructures, and LC biosensors that make use of LC and nanostructure characteristics.

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