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List of Poster Contributions

- | | | |
|---------------|---|---|
| Poster
9) | Silvia Pieraccini,
Maria Irene Donnoli,
Alberta Ferrarini,
Giovanni Gottarelli,
Giulia Licini,
Carlo Rosini,
Stefano Superchi
and Gian Piero Spada | DETERMINATION OF THE ABSOLUTE
CONFIGURATION
OF ALKYL ARYL SULFOXIDES
FROM NEMATIC DOPING EXPERIMENTS |
| Poster
10) | M.G. Clerc,
A. Petrossian,
S. Residori,
C. S. Riera | First-Order Fréedericksz transition and front
propagation in a
Liquid Crystal Light Valve with feedback |
| Poster
11) | A. Petrossian,
S. Residori
and L. Gil | Sum-frequency generation in dissipative systems:
experimental evidence for optical wave patterns |
| Poster
12) | Roberto Berardi,
Matteo Ricci,
and Claudio Zannoni | Bilayered Mesophases From Tapered Molecules. |
| Poster
13) | Geoffrey R. Luckhurst
and Katsuhiko Satoh | Molecular dynamics simulation
for the field-induced alignment of a smectic A phase |
| Poster
14) | R. Termine
and A. Golemme | MODELLING INDEX MODULATION
IN PHOTOREFRACTIVE CHIRAL SMECTIC
PHASES |
| Poster
15) | Carlo Versace,
Giuseppe Strangi,
Nicola Scaramuzza,
Vincenzo Bruno. | Electrically Induced Turbulence in
Nematic Liquid Crystal Layers |
| Poster
16) | Toshikuni MIYAZAKI
and
Mamoru YAMASHITA | Ordering and Molecular Bend at Gay-Berne Model |
| Poster
17) | Satoshi TANAKA
and
Mamoru YAMASHITA | Correlation Functions at Antiferroelectric Smectics
by Means of Transfer Matrix Method |
| Poster
18) | MASAFUMI YOSHIDA
and
HIROKAZU TORIUMI | Generalized Lennard-Jones Potential
for Molecular Simulation of Liquid Crystals |

Poster

ROLE OF THE N~N BRIDGE LENGTH OF THE SALEN-LIKE LIGANDS ON THE MESOMORPHIC PROPERTIES OF METAL COMPLEXES

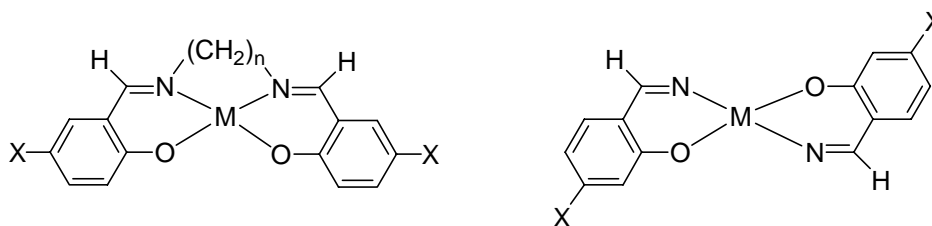
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Metallomesogens are metal-containing liquid-crystalline compounds¹ whose thermotropic properties depend on the metal ion coordination sphere and on the geometrical features imposed by the surrounding.

The salen-like ligands are versatile compounds from which several calamitic metallomesogens have been prepared. 2,3 The common structural features of these species (I) were: i) $n = 2$ or 3 for the $-(CH_2)_n-$ spacer; ii) the flexible tails X placed in position 5 and 5' and iii) the metal coordination geometry N,N cis.

The present investigation (II: $n = 12$; $M = Ni(II), Cu(II)$) proves that liquid crystalline materials (smectic or nematic) are obtained even when the elongated X group is in position 4 provided that $-(CH_2)_n-$ is large enough to allow the N,N trans configuration.



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Poster

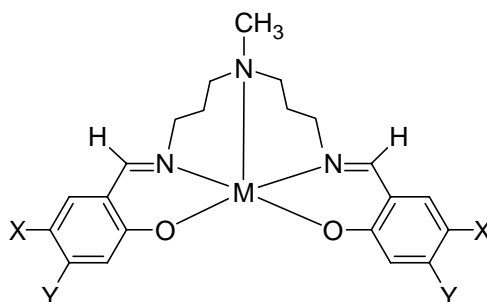
THERMOTROPIC MESOMORPHISM IN PENTA AND HEPTACOORDINATED METAL COMPLEXES

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Most liquid crystalline transition metals complexes (metallomesogens) have been found to exhibit a square planar coordination geometry¹ while those with coordination number (c. n.) exceeding four are limited to few octahedral species.^{2,3} Moreover, examples of metallomesogens wherein the metal centre shows an odd c.n. are quite rare and almost unknown.

The molecular geometry imposed by the metal coordination sphere can be an useful synthetic tool to obtain mesomorphic species with unusual molecular shape and related unexpected physical properties. In order to explore the influence of the metal c.n. on the thermal behaviour, we have considered pro-mesogenic chelating ligands provided of a pentadentate cavity. Upon reaction of these ligands with Ni(II) or UO₂(II) salts the corresponding complexes (I) have been obtained and characterised for mesomorphism by optical microscopy, DSC and XRD. To the best of our knowledge, these species are the first pentacoordinated Ni(II) and heptacoordinated UO₂(II) metallomesogens reported up to now. Moreover, a comparison between the new pentacoordinated Ni(II) complexes and the previously synthesised tetracoordinated ones⁴ show that on changing the coordination environment, interesting differences are induced on mesomorphism.



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Poster

New LC Polymers and Block Copolymers Carrying Fluorinated Side Groups via ROMP

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Block copolymers, in which at least one of the polymer block constituents contains mesogenic groups, can present two types of order over different length scales. In fact, the supramolecular order of the phase separated blocks can coexist with the molecular order of the LC units in the same chemical structure of an LC block copolymer [1].

Among the available living polymerization methods for the preparation of block copolymers, the ring opening metathesis polymerization (ROMP) is suitable to produce well defined polymers and block copolymers from cyclic olefins [2]. While ROMP has previously been used for the preparation of polymers from typical LC monomers [3], in this work we have applied it to the synthesis of the first examples of LC polymers and block copolymers from norbornenes carrying fluorinated side-group mesogens (Figure 1). Fluorocarbon chains are special mesogens as their rigid rodlike character and hydrophobic/lipophobic nature make them self-assemble in phase separated smectic structures, even in the absence of other normal components of LC molecules [4].

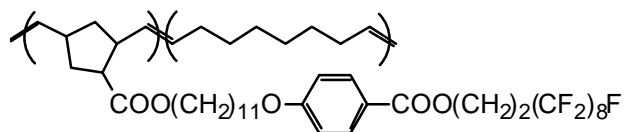


Figure 1. Example structure of LC block copolymer as prepared by ROMP.

The polymers were prepared from fluorinated norbornenes, and the block copolymers were prepared by sequential ROMPs of a norbornene and either a norbornene or a cyclooctene. Mo-carbene catalysts of the Schrock-type were used [5]. The synthesis of the polymers will be presented and their mesophase properties will be discussed with particular reference to the phase separated LC block copolymers.

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Poster

An auto-aligned photopolarimeter

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A new auto-aligned photopolarimeter, that will be used to probe a liquid crystal(LC) cell, is described. As the LC cell is rotated, it steers the probing laser beam and the photopolarimeter head must be re-aligned to allow for this. To efficiently collect data this re-alignment must be done automatically. We show that using a quadrant photodetector and a two dimensional duo-lateral position sensing detector (PSD) it is possible to dynamically re-align the head..

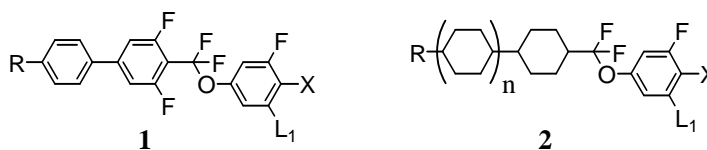
Poster

**SYNTHESIS AND PROPERTIES
OF NOVEL LIQUID CRYSTALLINE COMPOUNDS
HAVING A DIFLUOROMETHYLENEOXY MOIETY
AS A LINKAGE GROUP**

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Physical properties of the liquid crystalline materials currently required for the active matrix liquid crystalline displays (AM-LCDs) are lower driving voltage and lower viscosity, which induce the quick response characteristics of the displays.



To obtain materials that satisfy the above requirements, we have prepared the compounds (1) and (2) having the difluoromethyleneoxy (CF₂O) moiety as the linkage group, and measured their physical properties.[1] Due to the introduction of the CF₂O moiety in the molecules, the novel compounds exhibit the wider nematic temperature ranges, the greater dielectric anisotropy and the lower viscosity compared to the ordinary liquid crystal materials. (TABLE) As well as the advantageous physical properties, the novel compounds show excellent chemical stability. Therefore, we come into the result that the developed compounds are suitable as the components for the AM-LCDs currently desired. The synthesis and the detailed physical properties of the series of the novel compounds will be discussed.

TABLE Physical properties of the compounds (1) and (2) [a]

	<i>n</i>	R	X	L ₁	Mesophase (°C)	T _N (°C)	Δε	Δ <i>n</i>	γ ₁ (mPa · s)
1a	–	C ₆ H ₇	F	F	C 47.01	–16.4	22.3	0.125	63.3
1b	–	C ₆ H ₇	F	H	C 40.91	1.1	16.8	0.135	77.8
1c	–	C ₆ H ₇	OCF ₃	H	C 38.71	14.6	19.3	0.135	108.8
2a	0	C ₆ H ₁₁	F	F	C -0.61	–63.9	7.8	0.035	–94.2
2b	1	C ₆ H ₇	F	F	C 42.9 N 105.51	99.6	9.8	0.070	184.8
2c	1	C ₆ H ₇	F	H	C 35.6 N 129.01	125.6	6.3	0.070	212.3
2d	1	C ₆ H ₇	OCF ₃	H	C 32.0 N 136.51	125.1	8.3	0.080	242.8

[a] Clearing points (T_N), dielectric anisotropy (Δε), birefringence (Δ*n*), and rotational viscosity

(γ₁) are extrapolated data at 20°C, 20wt% in a liquid crystal mixture FB-01 (Chisso Corp., NI: 112.6°C, Δε: 4.8, Δ*n*: 0.080, γ₁: 171.3 mPa · s).

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Poster

A COMPUTER SIMULATION STUDY OF MESOPHASES FROM DIPOLAR BANANA-SHAPED MOLECULES

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We report the results of a Monte Carlo (MC) computer simulation of a system of $N=1000$ banana-shaped molecules with dipolar interactions. The banana-shaped molecule is modelled by joining three Gay-Berne sites with a bending angle of 120 degree; the dipole is located in the central site and oriented along the molecular x axis. We have investigated several temperatures corresponding to nematic and smectic liquid crystal phases in the isobaric-isothermal (NPT) ensemble, paying attention to the characterization of the smectic phase. At low temperature an untilted smectic phase with large biaxiality is found. Each smectic layer show local polarization, but layers are arranged in an antiferroelectric fashion and the overall sample is not polarized.

Poster

Topological Defects in Schlieren Textures of Biaxial and Uniaxial Nematics

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Monte Carlo and theoretical studies of thin 3D films of biaxial and uniaxial nematics with tangential boundary conditions show distinct differences in structure and evolution of topological defects. In the uniaxial films, defects of strength $k = \pm 1$ are point defects that bear no bulk singularity and disappear by annihilation with each other. In the biaxial films, $k = \pm 1$ defects are true singular bulk disclinations that split into pairs of $k = \pm 1/2$ lines; the latter disappear by annihilation processes of the type $+1/2 - 1/2 = 0$. These observed differences are of relevance for the current debate on the existence of biaxial phases.

Poster

Nematics with dispersed polymer fibrils: A Monte Carlo study of the external field-induced switching

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We present a Monte Carlo study of molecular ordering in nematics with dispersed regular and random arrays of straight and distorted polymer fibrils. We focus on the collective molecular reorientation --- the switching --- resulting from the competing aligning effects of fibrils and of a progressively applied transversal electric field, and identify structural Freedericksz and saturation transitions. The role of fiber topography in the switching behavior is monitored by simulating electric capacitance: slightly distorted fibrils are shown to give a sharper switching.

Poster

DETERMINATION OF THE ABSOLUTE CONFIGURATION OF ALKYL ARYL SULFOXIDES FROM NEMATIC DOPING EXPERIMENTS

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Despite the recognized importance of enantiopure sulfoxides as synthetic intermediates or auxiliaries in asymmetric synthesis [1], reliable and general methods for configurational assignment of these compounds are still lacking. CD spectroscopy in the framework of the "coupled oscillator" has been recently proposed [2] to assign the configuration of alkyl aryl sulfoxides, however this treatment can be rigorously applied only to sulfoxides where the aromatic ring and the SO group are not conjugated (such as alkyl 1-naphthyl compounds).

When doping a nematic phase with chiral nonracemic compounds, the molecular chirality is mapped onto the nematic phase by inducing a helical spatial arrangement of the nematic director. The magnitude and the sign of the induced pitch are related to the configuration and structure of the chiral dopant, and this allows empirical and rational correlation between molecular and phase chirality [3,4].

A series of (S)-alkyl aryl sulfoxides has been used as chiral dopants of the nematic phase E7: in all cases left-handed (M) twisted nematics are obtained. The sign and the magnitude of the helical twisting power have been calculated by the Surface Chirality model: the results are in good agreement with the experimental data. This approach appears to be a promising technique in assessing absolute configuration of chiral sulfoxides.

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Poster

First-Order Fréedericksz transition and front propagation in a Liquid Crystal Light Valve with feedback

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Liquid crystals under the influence of electric and magnetic fields exhibit a large variety of complex dynamical behavior, like electro-convection, pattern formation [1] and optical instabilities [2]. One of the most well-studied phenomena in the physics of liquid crystals is the field-induced distortion of a nematic liquid-crystal film, called the Fréedericksz transition (FT) [3]. For a nematic film, FT is usually a second-order transition [4]. In this communication, we show that FT becomes first-order for a planar aligned nematic film in which a feedback mechanism leads to a dependence of the applied electric field on the liquid crystal director. Experimentally, we realize this feedback by means of a Liquid Crystal Light Valve (LCLV) [5]. In the LCLV a nematic film is sandwiched between a glass and a photoconductive plate, which provides a conversion of optical intensity (changing with the liquid crystal re-orientation) into electric field (changing the liquid crystal orientation). Thus, an optical feedback loop can be designed in a such a way that the effective voltage drop across the nematic film depends on the liquid crystal orientation.

We explain the transformation of the FT into a first-order transition from fundamental principles, starting from the classical description in terms of the Frank free energy [6]. Close to the FT, we derive an amplitude equation which shows that, depending on the mutual orientation of the light polarization and the liquid crystal director, the FT can become first-order. Our theoretical description is in a fair qualitative agreement with the experimental observations. Depending on the values of the feedback parameters, both theory and experiment exhibit bistability, propagation of fronts and a Maxwell point. Experimentally, we have determined the hysteresis region, the Fréedericksz transition point and the Maxwell point. In one and two spatial dimensions, we have investigated the propagation of the fronts connecting the stationary states. In particular, in one dimension we have measured the velocity of front propagation.

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Poster

Sum-frequency generation in dissipative systems: experimental evidence for optical wave patterns

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Secondary instabilities of stationary patterns have been widely studied and reported in many experimental systems [1]. On the basis of symmetry arguments, it is possible to account for the spatial period doubling as the most common situation observed for stationary patterns [2]. In the case of traveling waves, any mechanism of secondary instability should imply a resonance condition not only for the spatial wavelengths but also for the temporal frequencies associated to the basic modes [3]. In close analogy with conservative systems, such as the nonlinear optics and the plasma physics, we have proposed a secondary instability mechanism, which is based on a three-wave interaction. For dissipative systems, the primary wave is the issue of the first bifurcation. Once developed, the primary wave gives rise to two generated waves, at upper and lower frequencies. Either the sum or the difference of the spatial and temporal frequencies of the two generated waves matches the frequency of the primary wave [4,5].

We have verified our theoretical predictions in an experiment based on a Liquid-Crystal-Light-Valve (LCLV) with optical feedback. We have introduced a ring shaped mask inside the cavity, so that the system is quasi-one dimensional satisfy periodic boundary conditions. This allows a direct comparison with the model. Moreover, a rotation of the feedback image corresponds to a shift along the ring and leads to the appearance of travelling waves when the input intensity exceeds the threshold for the primary bifurcation.

For the fixed experimental parameters the primary waves is composed of 43 cells along the ring. The inner diameter of the ring is $L = 5$ mm. By increasing the input intensity we observe a secondary instability characterized by the simultaneous appearance of smaller and larger cells, of wave number $(2\pi/L) \times 60$ and $(2\pi/L) \times 17$, respectively. Thus, we have $q_1 + q_2 - q_3 = 0$ where q_1 is the wave number of the primary wave and q_2 and q_3 are the wave numbers of the two generated waves. At the same time the dispersion relation is satisfied and the temporal frequencies are resonant, so that the relation $\omega_1 + \omega_2 - \omega_3 = 0$ is verified.

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Poster

Bilayered Mesophases From Tapered Molecules.

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The understanding of molecular factors that could lead to a specific mesophase organization, is a goal of great interest. Here we develop a simple molecular model [1] for non-centrosymmetric molecules. With suitable parametrisations of both shape and interaction part of this model potential we were able to obtain an interesting mesophase behaviour, i.e. a fluid bilayer structure.

We present results of Monte carlo (MC) computer simulation in the isobaric-isothermal ensemble (NPT) for single component systems of 8196 tapered molecules with three interaction-type parameters. We show how the combined effect of shape and interaction anisotropy could lead to the desired collective behaviour, and how the interaction anisotropy can play a central role in both the long and short range.

Poster

Molecular dynamics simulation for the field-induced alignment of a smectic A phase

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The nature of dynamics on the field-induced alignment of a smectic A phase have been investigated by a deuterium NMR [1, 2] and X-ray scattering [3] experiments recently. To help understand the complicated alignment process for the molecules as well as the director and the layer normal, we have undertaken a computer simulation of a system which is analogous to that of the real experiment. Our study of the alignment process for model mesogens would be expected to provide useful information on the dynamics as well as the structural properties at the molecular level. We have investigated the properties during the field-induced alignment process for a smectic A phase using a constant-pressure and constant-temperature molecular dynamics simulation for the Gay-Berne mesogen GB(4.4,20.0,1,1) with conventional three dimensional boundary conditions. Mainly systems with 4000 and 8788 particles have been used in these simulations. The dynamics of the alignment process has been explored using different angles between the director and the field applied as well as at different temperatures. For the case of 45°, which is between the initial angle between the director and the applied field, the molecules are found to be aligned smoothly to the field without destroying the layer structure which is in good agreement with the results of recent X-ray scattering experiment [3]. We also discuss the important relationship between the initial geometry for the particles and the angle applied.

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Poster

MODELLING INDEX MODULATION IN PHOTOREFRACTIVE CHIRAL SMECTIC PHASES

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The photorefractive effect is based on the photogeneration of mobile charges under non-uniform illumination: the charges redistribute in space by diffusion and eventually field induced drift and generate the so-called space-charge electric field. If the refractive index of the material is field dependent, the net effect is a phase shifted refractive index replica of the initial illumination pattern. In the field of organic photorefractive materials it has been realized that contributions to the index modulation due to birefringence are of paramount importance and this led the way to the development of liquid crystalline photorefractive materials, in which birefringence is high and spontaneous.

Because of their high refractive index anisotropy and low working voltages, photorefractive materials based on liquid crystals have become the subject of different studies in recent years. They can be considered as a particular subset of organic photorefractive materials where the index modulation is due to the reorientation of the mesophase optical axis under the influence of the space-charge field. The first photorefractive mesophases were bulk nematics or dispersions of nematic domains in photoconducting polymers. More recently, reports of smectic mesophases with photorefractive properties have appeared^{1,2} where the director reorientation is not, as in nematics, a quadratic effect in the field due to dielectric anisotropy, but instead it is a linear response due to the interaction of the field with a spontaneous (ferroelectric) or induced polarization. The drive behind the development of such smectic photorefractive materials lays in their fast reorientation times, which can be in the range of 10 ms instead of the 1-10 ms typical of most nematic devices, although in photorefractive applications such short times have not yet been achieved.

In order to optimize the photorefractive performance of smectic materials it is necessary to understand how the index modulation depends on a variety of parameters. In this work we present a simple model to calculate the refractive index modulation associated with the director reorientation in photorefractive SA* and SC* phases. The model takes into account several material parameters, as well as the direction and the polarization of the incident beams. We first obtain the local director orientation under the simultaneous influence of an applied and a photogenerated electric field and we then complete the task of obtaining the refractive index modulation taking also into account the polarization and direction of the incident light and the orientation of smectic layers. A comparison with experimental data will be illustrated.

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Poster

Electrically Induced Turbulence in Nematic Liquid Crystal Layers

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During the last decade some progresses have been achieved in understanding the formation and the dynamics of electrohydrodynamic patterns in nematic liquid crystals [1,2]. In particular the transition between the two turbulent states called dynamic scattering modes (DSMs) has attracted the interest of a large number of scientist [3,4,5]. In this paper we report of our improvements in the comprehension of the phenomenon, in particular we related the onset of the transition to a sudden change in the ac current which flow trough the nematic cell, electrical and dynamic light scattering measurements are presented.

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Poster

Ordering and Molecular Bend at Gay-Berne Model

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It is an interesting problem how the liquid crystalline ordering depends on the shape of constituent molecule from which the anisotropy of interaction is determined. For example, the shape of the tail [1] and the bent of molecule [2] work a serious part in the order of antiferroelectric smectics.

In this study rather simple system is introduced to study the effect of the molecular bend to the ordering, where the molecular dynamics simulation is carried out. The molecule is a dimer of two types of Gay-Berne particles connected by harmonic spring at each end and makes a given angle at isolated state of energy minimum, about which the preliminary results are already reported. Here, decrease of clearing temperature with the increase of the bend angle of molecule is depicted. By changing the strength of the connecting spring, the relation of the ordering to the flexibility is also tested.

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Poster

Correlation Functions at Antiferroelectric Smectics by Means of Transfer Matrix Method

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In antiferroelectric smectics, various types of layer stacking appear because of a frustration among interactions, while the ordering within the layer is enough stiff [1,2]. So, the correlation along the layer normal direction is quite interesting [2,3].

In this study, the ANNNI model, with the nearest neighbour interaction J_1 and the second nearest neighbour one J_2 (< 0) along layer normal together with the nearest neighbour interaction J within the layer, is introduced to describe the frustration in the antiferroelectric smectics [4,5]. A revised transfer matrix method is utilized to analyse the pair-correlation functions, where the interaction within the layer is replaced by the molecular field. We calculate the correlation functions at ferroelectric phase (SmC^*), antiferroelectric phase ($SmCA^*$), ferrielectric phase ($SmCg^*$), another type of antiferroelectric phase (AF) and an intermediate one with period 6.

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Poster

**Generalized Lennard-Jones Potential
for Molecular Simulation of Liquid Crystals**

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In order to improve the applicability of pairwise model potential, an anisotropic Lennard-Jones function was expanded by taking consideration of molecular geometrical and electrical details, and its parameters were optimized by using the genetic algorithm. In this approach, the intermolecular potential between a pair of uniaxial molecules can be written as:

$$(1) \quad V(u_1, u_2, r, R) = \varepsilon(u_1, u_2, r) \left\{ \left(\frac{1}{R - \sigma(u_1, u_2, r)} \right)^{12} - \left(\frac{1}{R - \sigma(u_1, u_2, r)} \right)^6 \right\} \dots$$

where, $e(u_1, u_2, r)$ and $s(u_1, u_2, r)$ are determined by the mutual configuration of the two molecules (Fig.1), and are expanded as a series of u_1 , u_2 , and r . This formulation has enough number of parameters to be optimized to reproduce the intermolecular potential of highly anisotropic molecules, while the conventional Gay-Berne (GB) model has only four parameters. Figure 2 demonstrates that the potential function $V(u_1, u_2, r, R)$ given in eq. 1 can completely reproduce the intermolecular potential function of the LJ beads molecules for the four typical configurations, but that the conventional GB model can only partially reproduce them because of the lack of the parameters. It should also be noted that the model potential introduced in eq. 1 can be extended for linear beads molecules of arbitrary lengths, polar molecules and biaxial molecules. The parameter optimization for these systems can be performed for the intermolecular potential calculated by the latest multi-molecular ab-initio calculation.

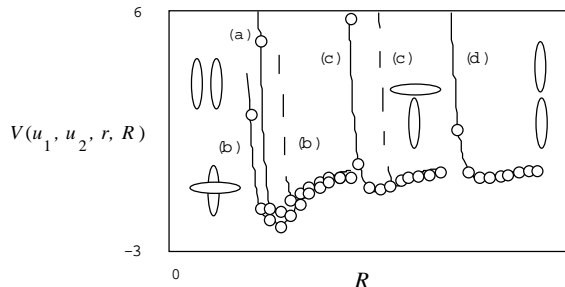
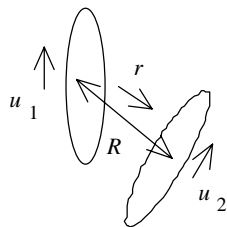


FIGURE 1 Generalized Lennard- Jones potential. Mutual configuration is expressed by u_1 , u_2 , and r . R is the distance between the centers of the mass.

FIGURE 2 Potential curves of the beads molecule for (a) side-by-side, (b) cross, (c) T-shape, and (d) end-to-end configuration. Circle: original potential of the LJ beads molecule, solid line: optimized generalized LJ potential, broken line: optimized conventional GB potential-