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Data-driven prediction of dielectric anisotropy in nematic liquid crystals

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ABSTRACT

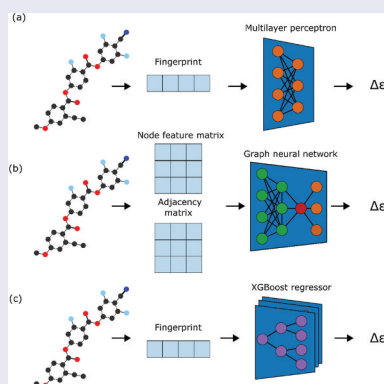
We curate a large-scale dataset of low frequency dielectric anisotropy values for low molecular weight liquid crystals. Using this dataset, we demonstrate that supervised machine-learning models can predict dielectric anisotropy with substantially improved accuracy (RMSE 2.6) compared to estimates obtained from the Maier-Meier relations using molecular properties from both the widely used semiempirical AM1 method (RMSE 9.7) and the modern r2scan-3c composite method (RMSE 11.2). Realising the potential of machine learning techniques for liquid crystalline materials requires carefully curated data to be accessible, and on this basis, we propose a simple and standard template for reporting data.

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Liquid crystals; nematics;
dielectric anisotropy;
machine learning



Introduction

Nematic liquid crystals are widely exploited in display technology, making the ability to accurately predict their macroscopic properties from molecular structure a central challenge in materials design. In contrast to other functional and soft materials, liquid crystalline materials must be synthesised in high chemical purity and are (typically) characterised as bulk materials in the condensed anisotropic state, rather than in dilute (isotropic) solution. As a result, experimental screening of materials is intrinsically low-throughput, time-consuming, and resource intensive. This creates a particularly acute need for accurate predictive structure-property relationships, especially tools and methods capable of linking molecular scale properties to measurable bulk properties. Of the many properties of nematic liquid crystals, the dielectric anisotropy ($\Delta\epsilon$) is of particular importance, governing electro-optic response,

switching behaviour, and device operating voltages. Dielectric anisotropy is often calculated according to the Maier-Meier relationship, effectively an extension of Onsager theory to anisotropic systems with long range orientational order, given in Equation (1):

$$\Delta\epsilon = \frac{NFh}{\epsilon_0} \left\{ \Delta\alpha - \frac{F\mu_{\text{eff}}^2}{2k_B T} (1 - (3\cos^2\beta)) \right\} S \quad (1)$$

Where $\mu_{\text{eff}}^2 = \sqrt{g \cdot \mu^2}$, μ is the molecular electric dipole moment, g is the Kirkwood g factor, β is the angle between the electric dipole moment and the molecular long axis, $\Delta\alpha$ is the anisotropic polarisability, N is the number density, F is the reaction field factor, and h is the cavitation factor which are defined according to:

$$F = \frac{1}{1 - \left(\epsilon - \frac{1}{(2\pi\epsilon_0 a^3) \cdot (2\epsilon + 1)} \right)} \quad (2)$$

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$$h = \frac{3\varepsilon}{(2\varepsilon + 1)} \quad (3)$$

The semi empirical AM1 method has been successfully used to calculate dielectric anisotropy from computed dipole moments and polarisability tensors [1–5]. Despite this empirical success, the AM1 method is known to significantly underestimate polarisability [6,7]; its apparent success when used with the Maier-Meier relations demonstrating that numerical agreement does not imply physical fidelity. More generally, while the Maier-Meier relation provides a mean-field link between computable (or measurable) molecular properties and macroscopic dielectric response, its underlying assumptions (single molecule response, weak treatment of intermolecular correlations) can restrict its quantitative accuracy.

Hybrid density functional theory (DFT) methods have been used with Maier-Meier relations with some success [8,9], yet the application of composite methods – which combine high chemical accuracy with low computational cost – remain unexplored. At the same time, the growing availability of chemically diverse datasets, together with rapid progress in (un)supervised molecular machine learning, raises the question of whether dielectric anisotropy can be predicted directly from molecular structure without reliance on explicit mean-field models.

Here we address this question using supervised machine-learning models trained to predict $\Delta\varepsilon$ of nematic liquid-crystalline materials. In the absence of any public dataset of experimental $\Delta\varepsilon$ data for individual molecules exists, we curated our own for this purpose, drawing from both academic and patent literature. Three machine-learning model architectures were trained: multilayer perceptron (MLP), graph neural network (GNNs) and XGBoost Regressor. The predictive performance of these models was benchmarked against dielectric anisotropies estimated using the Maier-Meier relation, employing both a widely used semi-empirical electronic-structure method (AM1) and a modern, low-cost composite density-functional approach (r^2 SCAN-3c). This comparison enables a direct assessment of data-driven and physics-based approaches for predicting dielectric response across chemically diverse liquid-crystal systems. Finally, Shapley additive explanations (SHAP) analysis is performed on the best performing fingerprint model to evaluate the relationship between descriptor values and $\Delta\varepsilon$ prediction.

Method

Dataset curation

We curated a dataset of low frequency dielectric anisotropy data for single component low molecular weight

liquid crystals. The dataset covers around 3500 unique molecular structures, drawn from both journal [10–129] and patent literature [130–503]. The dataset includes data measured for pure materials and that obtained by extrapolation from mixtures. The dataset does not include data for mixed systems (e.g. unextrapolated mixtures, mixtures of isomers, low purity materials). Where the same material was reported in multiple papers and/or patents, we use values from the earliest publication.

It is important to note that the dielectric anisotropy of a nematic liquid crystal is, in general, temperature dependent. This dependence arises primarily from the temperature dependence of the orientational order parameter, $\langle P_2 \rangle$, since $\Delta\varepsilon$ is governed by the projection of molecular dipole and polarisability anisotropy onto the nematic director. Other factors, including density and intrinsic molecular properties, are expected to vary only weakly over the temperature range in which conventional nematic phases are normally observed. In the present work, most $\Delta\varepsilon$ values are extrapolated from dilute mixtures in broad-temperature-range nematic hosts and are measured close to ambient temperature. These values should therefore be regarded as standardised comparative $\Delta\varepsilon$ values rather than full temperature-dependent $\Delta\varepsilon(T)$ datasets. The machine-learning models developed here are consequently intended to capture molecular structure-property relationships in these standardised experimental values, rather than to predict the temperature dependence of $\Delta\varepsilon$. Residual variation due to host, temperature, and order parameter effects is treated as part of the experimental uncertainty in the dataset.

Molecular structures were transcribed using a text-based notation system and represented as text using the simplified molecular input line entry system (SMILES). The raw dataset was handled using RDKit [504], allowing us to filter inadvertent duplicates due to human error (e.g. where two identical molecules have different ‘raw’ SMILES due to differing ring indices).

Electronic structure calculations

We converted SMILES strings into 3D coordinates using the ETKDGV3 (experimental-torsion-knowledge distance geometry) conformer generator [505] in RDKit (Release_2025.09.4). We then performed geometry optimisation and calculation of dipole moment and polarisability tensors using the AM1 semi-empirical method (Gaussian G16 [506]) and the r^2 scan-3c composite method [507] (Orca 6.1 [508]).

Dataset informatics

We computed descriptors (Molecular weight, fraction Csp [3]) using the Descriptors module in RDKit. Uniform manifold approximation and projection (UMAP) was performed with the UMAP-learn package [509] using Mordred fingerprints. Prior to embedding, descriptors containing non-finite values (NaN or ∞) were removed, and molecules with remaining non-finite entries were excluded. The cleaned descriptor matrix was embedded into two dimensions using UMAP with $n_neighbors = 20$, $min_dist = 0.1$, and a fixed random seed to ensure reproducibility.

Machine learning

Molecular fingerprints (1024 bit) were generated using the *skfp.fingerprints* Python package [510]. For three-dimensional fingerprints we generated low-energy conformers from the SMILES string using the ETKDGV3 algorithm in RDKit [504]. Machine learning models were trained using supervised learning framework using PyTorch [511]. The molecular fingerprints were used as the input, and the values of dielectric anisotropy as the target. The dataset was randomly divided into test/training sets using an 80:20 split. Model training was performed for 500 epochs (with early stopping) using the Adam optimiser with a learning rate of 1×10^{-3} and a weight decay of 1×10^{-4} . A batch size of 64 was employed throughout. Model performance was evaluated using 5-fold cross-validation on the training data. Predictive accuracy was assessed on the held-out test set. All fingerprint neural networks shared the same topology (Figure 1). Hyperparameter choice was made empirically based on the need to balance training stability and predictive performance.

Fingerprint-based multilayer perceptron (MLPs; Figure 1(a)) operate on fixed-length fingerprint vectors which encode molecular information. The MLPs learn to map to a target property through the transformations of successive hidden linear layers. Graph neural networks (GNNs; Figure 1(b)) instead are passed molecular graph representations and learn atomic-level representations through message-passing convolutional layers. These atomic-level representations are then pooled into a molecular-level prediction. As a non-neural-network comparison, the XGBoost regressor (Figure 1(c)) builds an ensemble of decision trees, each trained to correct the residual errors of the previous tree.

Molecular graph representations were produced using previously published code [512], and the models were trained according to the hyperparameters

described in the ESI. An XGBoost [513] regressor model was trained in a manner as to replicate the MLP training process. It was parameterised with 500 estimators, a max depth of 10, a learning rate of 0.01.

Results

Dataset analysis

Although the curated dataset is a broad cross-section of reported materials and design strategies, it is not (nor could it be) an exhaustive list of all possible materials nor all reported materials. By necessity, the present dataset is shaped by experimental accessibility, by academic interest, by commercial relevance, and by disclosure. The iterative optimisation around certain building blocks (e.g. fluorinated aromatics) leads to clustering. The dataset comprises ~43% materials with negative dielectric anisotropy ($N = 1542$, average $\Delta\epsilon = -6.7$; Figure 2(a)) and ~57% with positive dielectric anisotropy ($N = 2065$, average $\Delta\epsilon = +15.75$; Figure 2(a)). The average molecular weight across the dataset was 416 with a standard deviation of 118 (Figure 2(b)).

Molecules with large negative or positive values of $\Delta\epsilon$ typically feature a relatively modest fraction of saturated hydrocarbon; as the fraction of Csp [3] tends towards one the values of dielectric anisotropy cluster in the range 0–10. The dominant feature here is variance rather than trend (Figure 2(c)).

The chemical space within the dataset is highly structured giving the UMAP projection a filament-like appearance; positive and negative materials are broadly interspersed throughout this space, although in some regions a clear bias to one sign of $\Delta\epsilon$ can be seen (Figure 2(d)). However, as UMAP is a non-linear embedding optimised for *local* neighbourhood preservation, distances and apparent clusters within the projection should not be over interpreted.

Electronic structure calculations

Initial 3D geometries for dataset entries were generated from SMILES strings using the ETKDGV3 conformer embedding method in RDKit. Where the conformer embedding failed (typically due to a lack of parameters, e.g. for hypervalent sulphur in SF₅) the geometry was manually generated. Electronic structure calculations were performed using either the AM1 semiempirical method or the r2scan-3c composite method. For each molecule, and with each method, we perform geometry optimisation followed by a frequency calculation to confirm the absence of imaginary frequencies. We then compute the dipole vector and polarisability

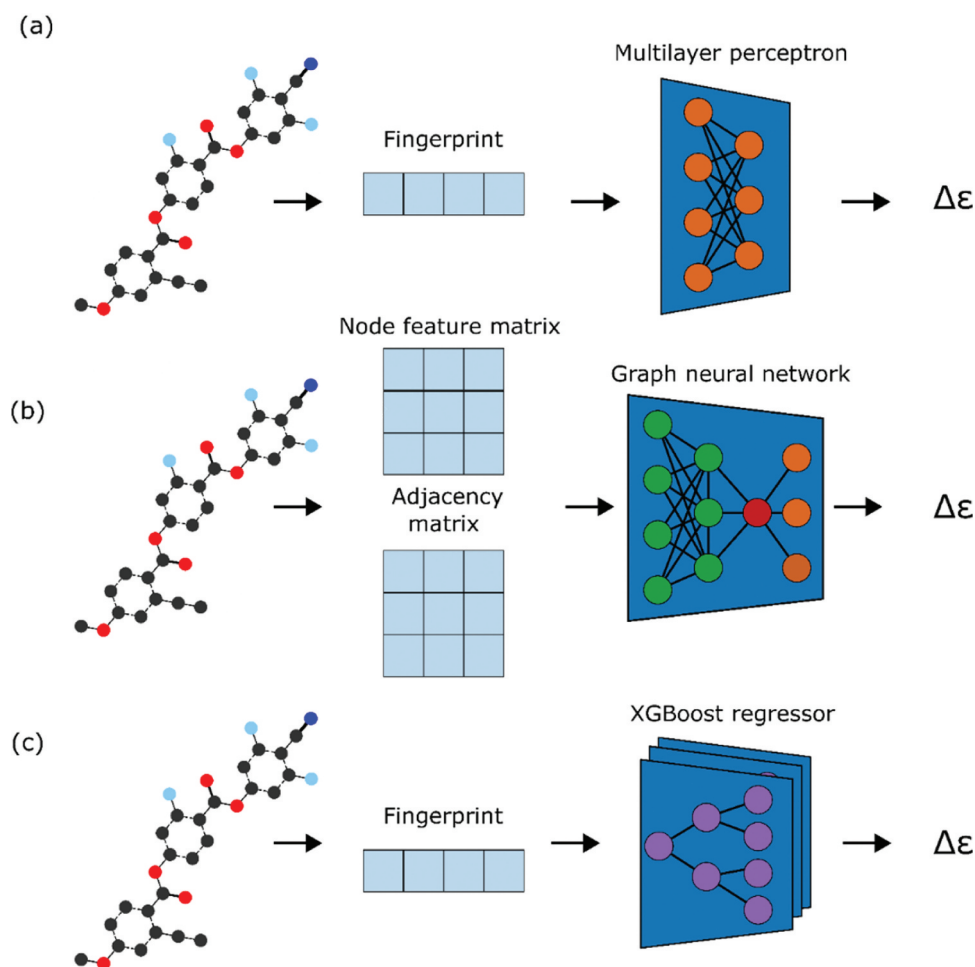


Figure 1. (Colour online) Schematic representation of the machine learning architectures used in this work. (a) illustrates the multilayer perceptron that transforms a molecular fingerprint through successive hidden layers to predict $\Delta\epsilon$. (b) Shows how a graph neural network where the molecule is represented by a node feature matrix and an adjacency matrix. The information of neighbouring nodes is aggregated through message passing layers (green), then pooled to a graph level representation (red). A scalar prediction is then produced through the linear transformation layers (orange). (c) depicts the XGBoost regressor in which an ensemble of decision trees predicts $\Delta\epsilon$ via sequential error correction.

tensor. Using the Maier-Meier relation with the obtained dipole and polarisability data with $S = 0.65$, $\rho = 1.00 \text{ g cm}^3$, $T = 298 \text{ K}$, and $g = 1$, we obtain the dielectric anisotropy.

In contrast to earlier use of the AM1 method for calculating dielectric anisotropy [1–5], the dataset used here is orders of magnitude larger. However, we find AM1 performs rather poorly: the root mean square error (RMSE) is 9.66 which corresponds to approximately 0.61σ of the experimental distribution ($r^2 = 0.632$; Figure 3(a)). While this is a moderate degree of correlation, the magnitude of error and presence of frequent sign errors (*vide infra*) limit the qualitative predictive utility of the AM1 method in a workflow for predicting dielectric anisotropy.

Modern composite DFT methods such as r2scan-3c offer high chemical accuracy with low computational

cost. That said, for our dataset we find an RMSE of 11.2 with the r2scan-3c method, corresponding to approximately 0.71σ of the experimental $\Delta\epsilon$ distribution ($r^2 = 0.500$; Figure 3b). This performance is notably worse than that of AM1, indicating that increased accuracy of the electronic structure calculation does not translate to an improved predictive accuracy for $\Delta\epsilon$ via the Maier-Meier relation.

Both AM1 and r2scan-3c have significant ‘sign errors’, where a material with negative $\Delta\epsilon$ is calculated to be positive (AM1: 10%, 297 entries; r2scan-3c: 13%, 371 entries) or a material with positive $\Delta\epsilon$ is calculated to be negative (both 3% of all entries). The poor performance of both methods presumably reflects the non-ideal use of the molecular ‘long axis’ for orientation, that the calculations are performed on an isolated molecule and extrapolated to the bulk, the neglect of conformers, variations in ρ , S , g and so on.

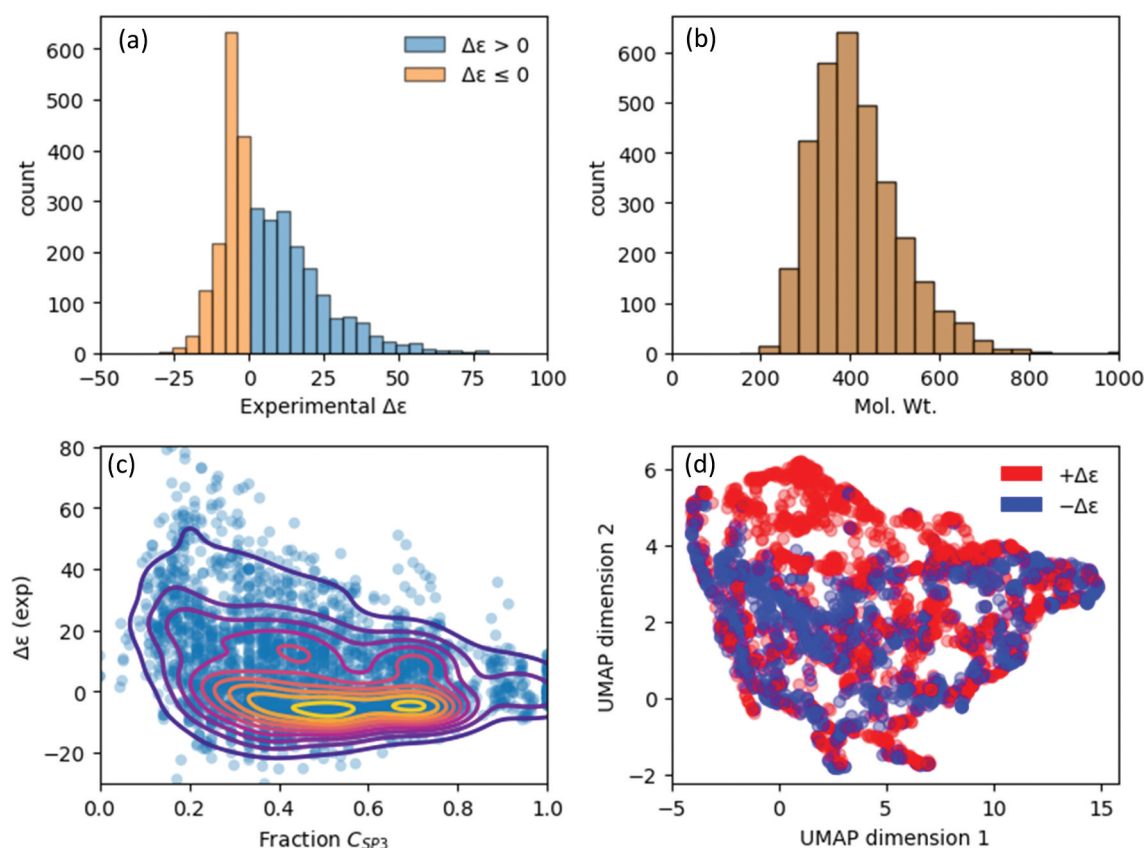


Figure 2. (Colour online) Analysis of the curated dataset. (a) Histogram plot of the reported values of dielectric anisotropy, coloured according to sign. (b) Histogram plot of molecular weight for molecules within the curated dataset. (c) Scatter plot of experimental dielectric anisotropy versus the fraction of the molecule comprising sp^3 hybridized carbon, where solid contours represent the estimate point density to highlight the regions of highest data concentration. (d) UMAP projection of Mordred molecular fingerprint descriptors, with points coloured according to the sign of dielectric anisotropy.

Considering multiple conformers may be a viable route to improving the accuracy of the calculated dielectric anisotropy. The computational cost of this is not negligible however; the optimisation and property calculations with r2scan-3c for the dataset took over 2700 CPU hours on a modern HPC system (Aire HPC at the University of Leeds). A back of the envelope calculation (assume 12 CPU hours to generate and optimise the conformers (using ORCA-GOAT) and consider just 10 conformers per molecule) would increase this to ~65800 CPU hours (around 7.5 CPU years), which is not insignificant.

Plotting the residual $\Delta\epsilon$ ($\Delta\epsilon_{\text{calc}} - \Delta\epsilon_{\text{meas}}$) versus the experimental value (Figure 3(c,d)) reveals a clear negative slope, especially pronounced for r2scan-3c; in other words, an anticorrelation between prediction error and magnitude of the experimental value. This is particularly pronounced for r2scan-3c, and indicates a systematic deviation from ideal scaling, with increasingly strong underestimation at large positive and negative $\Delta\epsilon$.

The residual distributions (Figure 3(e,f)) are approximately Gaussian but are shifted away from

zero and with moderate-to-large variance (standard deviation). The combination of non-zero mean and significant variance reflects the presence of systematic error in the results and significant uncertainty across the entire dataset (as opposed to a few problematic structures).

Taken together, these diagnostics demonstrate that while electronic structure methods capture qualitative trends in dielectric anisotropy, their errors are structured rather than random. The presence of systematic anticorrelation in residuals indicate that factors governing the magnitude of $\Delta\epsilon$ are not fully captured by the models, and this motivates the use of data-driven approaches which we now turn to.

Supervised machine learning

Supervised machine learning is well suited to learning structure-property relationships from these representations in cases where no simple analytical model exists. This is particularly relevant for dielectric anisotropy, which emerges from properties

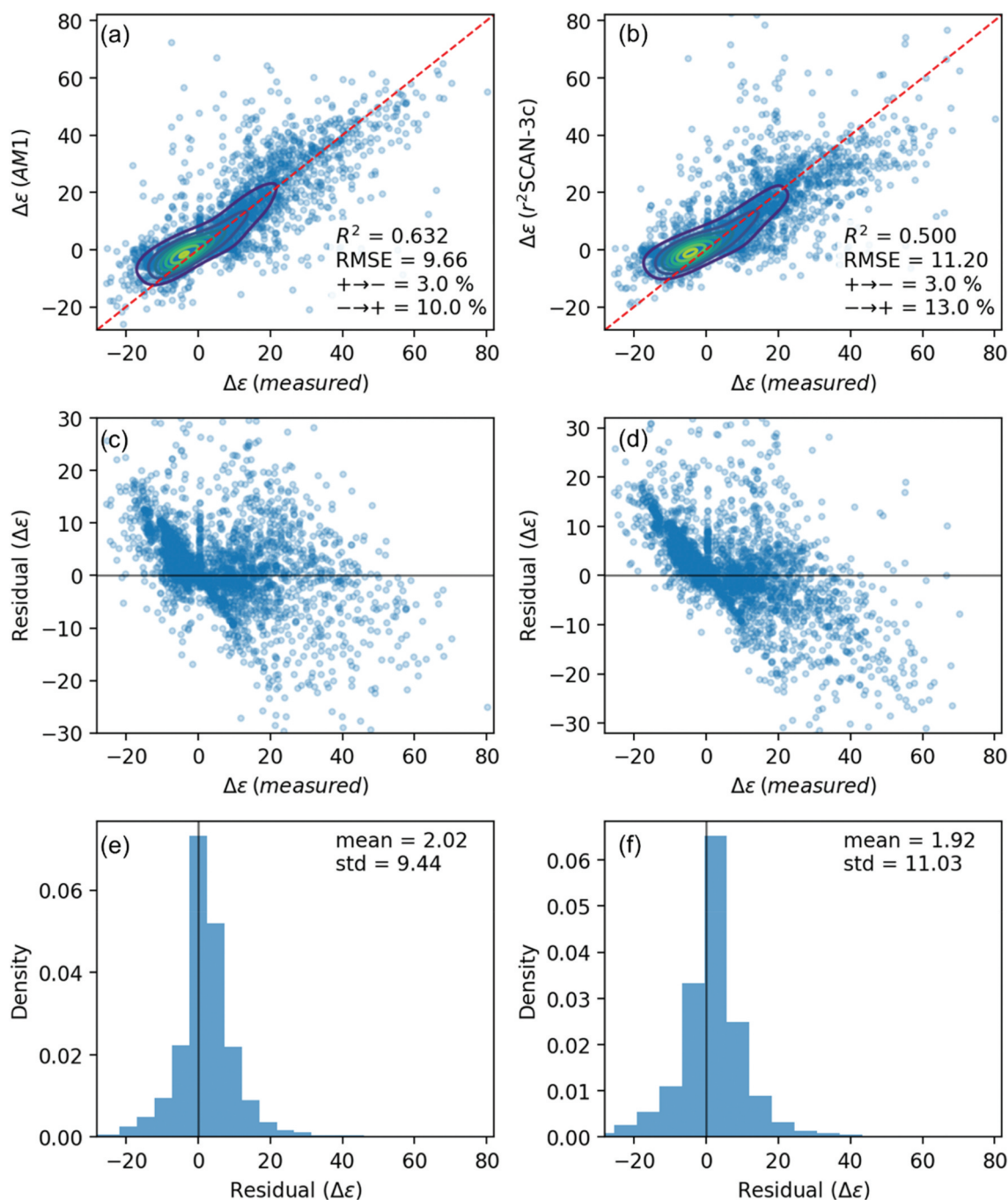


Figure 3. (Colour online) Plot of calculated (y) vs actual (x) dielectric anisotropy using geometry and properties from: (a) the semi-empirical AM1 method ($RMSE = 9.66$; $r^2 = 0.632$), and (b) the r2scan-3c composite method ($RMSE = 11.20$; $r^2 = 0.500$). Kernel density estimate (KDE) contours represent the estimated point density and so highlight the regions of highest data concentration. The dashed line represents perfect agreement (i.e. $x = y$). Both methods display significant sign inversions, as indicated by $+\rightarrow-$ (experimental $-\Delta\epsilon$, predicted $+\Delta\epsilon$) and $-\rightarrow+$ (experimental $+\Delta\epsilon$, predicted $-\Delta\epsilon$). Plots of residual vs actual $\Delta\epsilon$ for AM1 (c) and r2scan-3c (d). Histogram plot of residuals for AM1 (e) and r2scan-3c (f) with mean value and standard deviation labelled.

across a range of length scales from the molecule (polarity, polarisability, electronic structure etc) to the bulk (e.g. order parameter, density). The performance of different models using different input types is summarised below and shown graphically in Figure 4.

Molecular fingerprints provide a numerical representation of chemical structure, encoding atomic connectivity, functional groups, and, in some cases, physicochemical descriptors. Such representations are particularly well suited to statistical learning, as they map chemically diverse molecules onto a common,

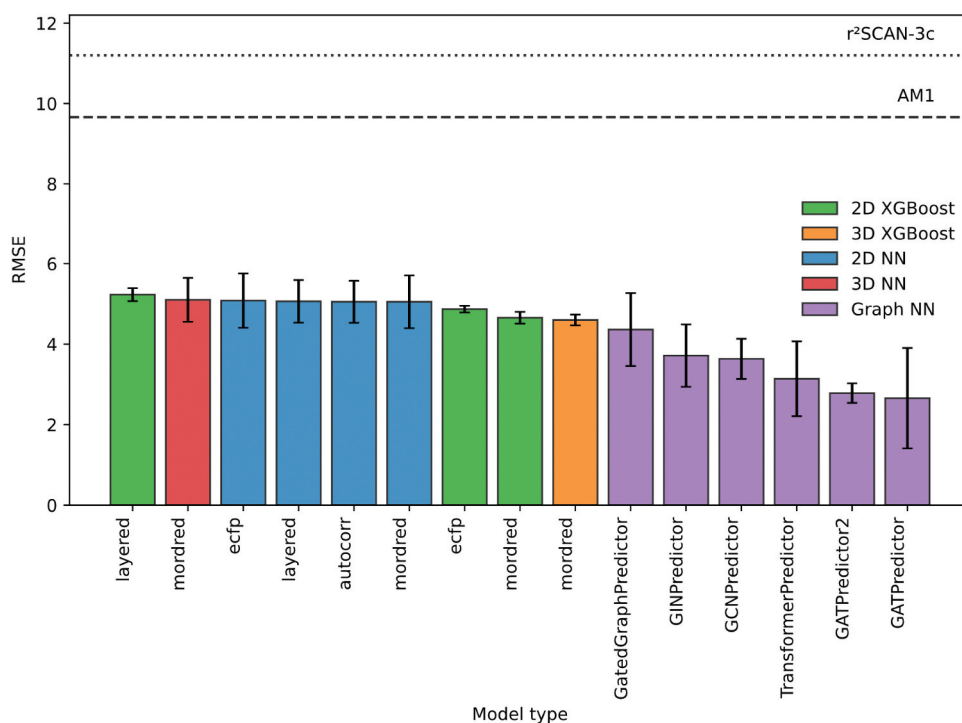


Figure 4. (Colour online) Performance of selected supervised machine-learning models for predicting dielectric anisotropy ($\Delta\epsilon$) to compare a) molecular fingerprint vs graph representations and b) neural networks vs. XGBoost regressors. Bars show the root-mean-square error (RMSE) on the independent hold out test set for each model type; error bars show the standard deviation of the RMSE across cross-validation folds, arising from the repeated data partitioning during model training. The bar colours indicate the input used to train the network (blue = 2D fingerprint, red = 3D fingerprint, purple = molecular graph, green = 2D XGBoost, orange = 3D XGBoost). Horizontal dashed lines indicate the RMSE obtained for the same dataset when computing using the maier-meier relations with molecular properties as computed with the AM1 semi-empirical and r2scan-3c composite methods (*vide supra*). Additional examples of less performant networks are given in the ESI to this article.

fixed-length feature space. In this work, multiple fingerprint representations were generated for each molecule, each of these being a 1024-bit vector, enabling direct comparison and regression across the full dataset.

Molecular graphs are a representation in which atoms are treated as ‘nodes’ and bonds as ‘edges’, preserving the topology of the molecule without reliance on predefined descriptors. Unlike fingerprints (which are fixed-length features), graph representations retain information about relations between atoms; they are well suited to statistical learning and preserving chemically meaningful features that derive from the underlying molecular connectivity and topology.

Three supervised machine learning approaches were employed to predict $\Delta\epsilon$ values. The MLP and the XGBoost models were trained on fingerprint representations, whereas the GNN models were trained on molecular graphs. Across all methods, test-set RMSE values ranged from 2.6 to 20.0. The *erg* and *usr* fingerprint types performed worse than calculations via AM1/r2scan-3c and using the Maier-Meier relations (both having $\text{RMSE} \geq 10$). We found 2D fingerprints to

outperform those using 3D geometries, even for the same fingerprint type (e.g. *AtomPair*, *Mordred*). Out of all fingerprints tested, 2D Mordred gave the lowest RMSE for the independent hold-out test set (4.8) although others (*Autocorr*, *Layered*, *ECFP*, *Mordred-3D*) had only fractionally higher RMSE. Our non-neural network comparison, XGBoost shows a slight outperformance of the MLP, with Mordred-3D, Mordred-2D and ECFP achieving RMSE values of 4.6, 4.7 and 4.9 respectively. The GNNs outperformed the fingerprint models in all cases, with the GATPredictor GNN achieving an RMSE of 2.6, again an improvement over the Maier-Meier relations

The parity plot for the best-performing fingerprint model (2D Mordred Fingerprints, Figure 5(a)) compares the predicted versus experimental dielectric anisotropy. The model reproduces the experimental values with r^2 of 0.91 and RMSE of 4.8, indicating that much of the variance in $\Delta\epsilon$ is captured by the learned representation. By these metrics, the network is far more accurate than the Maier-Meier relation utilising AM1 or r2scan-3c. Predictions are well distributed about the $x = y$ line

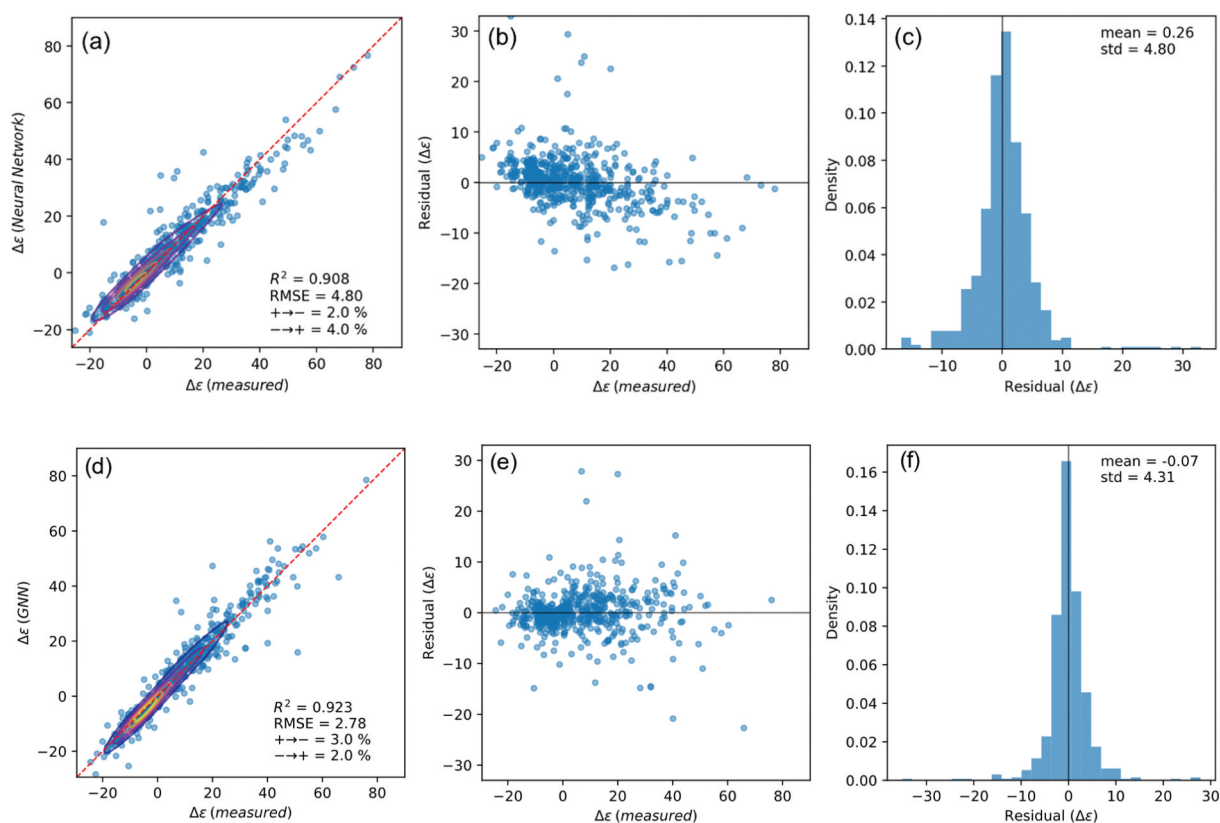


Figure 5. (Colour online) Fingerprint representation (top row) compared with graph representation (bottom row). Assessing the performance of the machine-learning model. Scatter plot of predicted $\Delta\epsilon$ versus experimental for the neural network trained against mordred fingerprints (a) and the GATPredictor2 model (d). Kernel density estimate (KDE) contours are overlaid to highlight the distribution of data density, together with the parity line (dashed). The coefficient of determination (R^2) and root-mean-square error (RMSE) are indicated. (b, e) residuals (predicted vs. measured $\Delta\epsilon$) plotted as a function of the experimental value, showing the absence of systematic bias across the range of dielectric anisotropies. (c, f) distribution of prediction errors for the independent hold-out test set, illustrating the spread and near-zero mean of the residuals.

across the full range of experimentally observed $\Delta\epsilon$ values with no evidence of systematic compression at high magnitudes. Encouragingly, the percentage of sign errors is far lower. The corresponding residuals (Figure 5(b)) have a much weaker tendency to underestimation at large positive or negative $\Delta\epsilon$. Importantly, no discrete regimes or discontinuities are observed which would indicate fingerprint-specific artefacts, if present. The histogram of residuals (Figure 5(c)) is Gaussian (to a first approximation) and centred close to zero (mean = 0.26, standard deviation = 4.80) which confirms the absence of systematic bias in the model.

Although the GATPredictor architecture achieved the lowest test-set RMSE, Figure 5 compares the Mordred-2D fingerprint model with GATPredictor2 results as this model achieved a lower standard deviation across its validation predictions (1.24 vs 0.24) which indicates a more stable model. GATPredictor2 achieves r^2 and RMSE values of 0.923 and 2.78 respectively. The parity plot (Figure 5(d)) shows a tighter clustering about the $y=x$ line and the residuals

(Figure 5(e)) present less of a break down in predictions at higher or lower $\Delta\epsilon$ values. This is quantified in Figure 5(f) where the residual distribution is calculated to possess a mean of -0.07 and a standard deviation of 4.31. Together, these results demonstrate that both molecular fingerprints and graph-based approaches can learn the structural property relationships that govern dielectric anisotropy values in a chemically diverse dataset, with GNNs possessing stronger performance metrics.

Finally, we use SHAP values to explore and interrogate the trained fingerprint model and identify which molecular descriptors most strongly influence the predicted value of $\Delta\epsilon$. SHAP values quantify the contribution of each descriptor to an individual prediction relative to the global model baseline. Positive SHAP values indicate features that increase the predicted dielectric anisotropy, whereas negative values correspond to descriptors that suppress it. Figure 6 presents a summary plot in which each point represents a single molecule, positioned according to the magnitude and direction of the

descriptor's impact. Points are coloured by the normalised descriptor value, allowing the relationship between feature magnitude and model response to be visualised directly.

In this analysis we identify a set of high-impact descriptors spanning multiple physiochemically meaningful families. Prominent among these were topological autocorrelation metrics such as GATS4s, GATS3C, MATS5c, and ATSC0pe, which encode how electronic properties are distributed across the molecular graph. Surface-area descriptors partitioned by charge and lipophilicity (including EOE_VSA12, EState_VSA4, EState_VSA2, and SLOGP_VSA4) were likewise strongly represented, indicating that the exposure and spatial segregation of polar surface is important in governing $\Delta\epsilon$.

Extremal electro-topological descriptors (MINssCH2, MINsCH3, MAXaasC) and graph-based invariant descriptors such as MIC4 and MDEC-11

highlight the importance of electronically differentiated atomic environments and overall molecular topology. While individual descriptors do not map uniquely onto specific chemical fragments, the convergence of these independent feature classes on electrostatic distribution provides a physically coherent interpretation of the model. Collectively, the results indicate that dielectric anisotropy is governed primarily by the spatial organisation of electronic character rather than dipole magnitude alone, which we feel aligns with common intuitive understanding of this property.

Machine learning can only be successfully deployed where curated data is available. In the present case, this required careful curation of a large-scale dataset spanning many journal articles and patents, coupled with transcription of chemical information into machine readable format. We would strongly encourage the inclusion of 'machine readable' data in the ESI of future

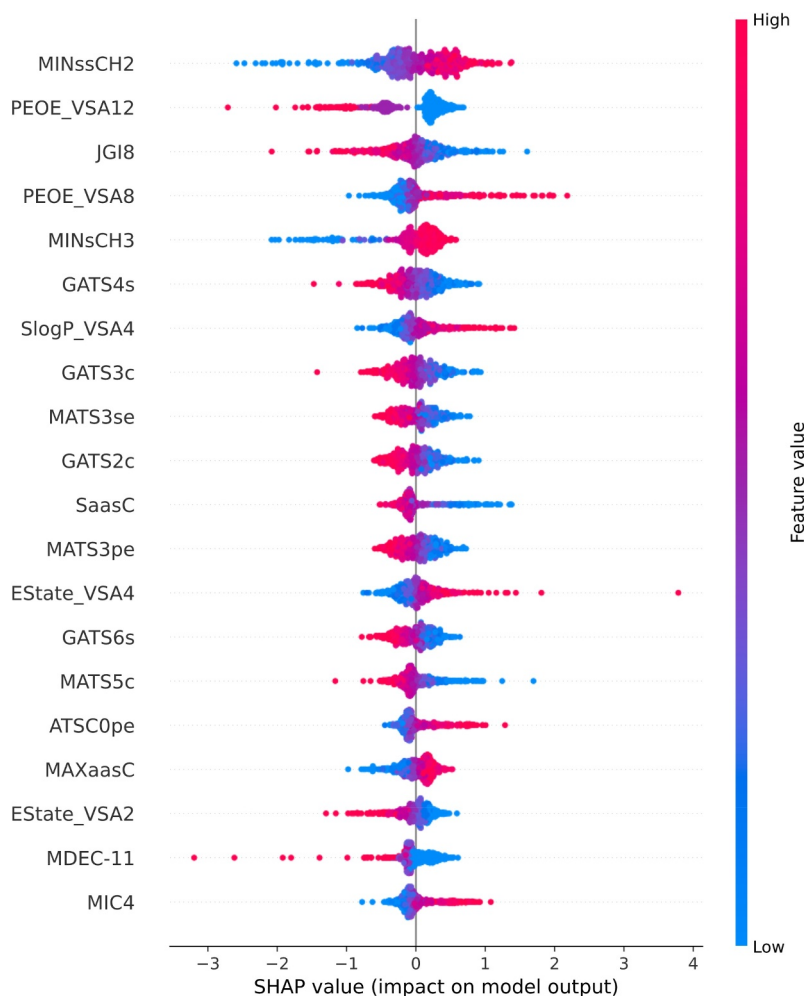


Figure 6. (Colour online) Calculated *SHapley additive exPlanations* (SHAP) values for the best performing fingerprint neural network model. Descriptors within the mordred fingerprint are ranked from most important (top) to least (bottom). Each point represents a unique molecule within the dataset. The colour scale reflects the normalised value of the descriptor value for each molecule. The position on the x-scale reflects the impact on the prediction of $\Delta\epsilon$.

papers, and we give an example of this in the ESI to this article using examples from the dataset in this work. This need is especially acute for chemical structures; it is commonplace to use 'X/Y/Z/R' groups and denote changes to structure in tabular form, and extracting the requisite information from data presented in this way is rather time consuming.

The present work complements prior use of machine learning methods in liquid crystal science such as classification of ferroelectric nematic materials [514], predicting clearing points [515,516], phase transitions in bent-core type materials [517], lyotropic phase behaviour [518], image-based frameworks for phase identification via optical texture analysis [519,520], hydrodynamic properties via director field dynamics [521], optimisation of LCD backlight technology [522], and data-led design of de novo ferroelectric nematics [512]. Together, these studies highlight the growing importance of machine learning in understanding liquid crystalline materials and devices.

Conclusions

While physics-based models such as the Maier–Meier relation provide invaluable conceptual insight, their predictive performance is ultimately constrained by both their underlying assumptions and the accuracy with which molecular properties can be computed. We show these limitations to become particularly acute when such approaches are applied across large, chemically diverse datasets. In contrast, the machine-learning models reported here achieve substantially improved predictive accuracy without explicit recourse to mean-field assumptions. Notably, the most accurate predictions are obtained without explicit modelling of intermolecular correlations or nematic order. Although such omissions may appear conceptually unsatisfying, they do not diminish predictive performance. From a materials-design perspective, predictive accuracy is therefore the most relevant currency.

Acknowledgments

Both RJM and CPB contributed to the conception and design of the work. RJM curated the dataset, which underwent checking by both RJM and CPB. Electronic structure calculations were performed by RJM. The machine learning code was written by both RJM (fingerprints) and CPB (GNNs, XGBoost). The manuscript was written by both RJM and CPB. Both authors agree to be accountable for all aspects of the work.

Author contributions

CRedit: **Charles Parton-Barr:** Data curation, Formal analysis, Investigation, Methodology, Software, Validation,

Visualization, Writing – original draft, Writing – review & editing; **Richard. J. Mandle:** Conceptualization, Data curation, Formal analysis, Funding acquisition, Investigation, Methodology, Project administration, Resources, Software, Supervision, Validation, Visualization, Writing – original draft, Writing – review & editing.

Disclosure statement

No potential conflict of interest was reported by the author(s).

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Data availability statement

The curated dataset of dielectric anisotropy values and molecular structures, code for training machine learning models, analysis code, and code used to generate figures is available via GitHub: https://github.com/RichardMandle/ML_dielectric.

References

- [1] Xu J, Okada H, Sugimori S, et al. Numerical evaluation of the relative value of dielectric anisotropy and order parameter in fluorinated nematic liquid crystals. *Jpn J Appl Phys.* 2001;40(3R):1375. doi: 10.1143/JJAP.40.1375
- [2] Klasen M, Bremer M, Götz A, et al. Calculation of optical and dielectric anisotropy of nematic liquid crystals. *Jpn J Appl Phys.* 1998;37(8A):L945. doi: 10.1143/JJAP.37.L945
- [3] Zhang R, He J, Peng Z-H, et al. Calculating the dielectric anisotropy of nematic liquid crystals: a reinvestigation of the Maier–Meier theory. *Chin Phys B.* 2009;18(7):2885.
- [4] Ma H, Sun R-Z, Li Z-X, et al. Temperature dependence of ratio between dielectric anisotropy and order parameter in fluorinated nematic liquid crystals. *Chin Phys B.* 2008;17(1):255.
- [5] Saitoh G, Satoh M, Hasegawa E. Estimating dielectric anisotropy of liquid crystal compounds. *Mol Cryst Liq Cryst Sci Technol Sec.* 1997;301(1):13–18. doi: 10.1080/10587259708041743
- [6] Hinchliffe A, Nikolaidi B, Soscún Machado HJ. Density functional studies of the dipole polarizabilities of substituted stilbene, azoarene and related push-pull molecules. *Int J Mol Sci.* 2004;5(8):224–238. doi: 10.3390/i5050224
- [7] Welborn M, Chen J, Wang L-P, et al. Why many semi-empirical molecular orbital theories fail for liquid water and how to fix them. *J Comput Chem.* 2015;36(12):934–939. doi: 10.1002/jcc.23887

- [8] Januszko A, Kaszynski P, Wand MD, et al. Three-ring mesogens containing p-carboranes: characterization and comparison with the hydrocarbon analogs in the pure state and as additives to a ferroelectric mixture *J Mater Chem*. 2004;14(10):1544–1553. doi: [10.1039/b311140g](#)
- [9] Mandle RJ, Cowling SJ, Sage I, et al. Relationship between molecular association and re-entrant phenomena in polar calamitic liquid crystals. *J Phys Chem B*. 2015;119(7):3273–3280. doi: [10.1021/jp512093j](#)
- [10] Dubois JC, Zann A, Couttet A. Tolanes nematiques. *Mol Cryst Liq Cryst*. 1974;27(1–2):187–198. doi: [10.1080/15421407408083129](#)
- [11] Van Meter JP, Klingbiel RT, Genova DJ. Dielectric properties of several liquid crystalline esters. *Solid State Commun*. 1975;16(3):315–318. doi: [10.1016/0038-1098\(75\)90176-3](#)
- [12] Bolotin BM, Zeryukina LS, Safina RU, et al. Liquid-crystal 4H-3,1-benzoxazln-4-ones. *Chem Heterocycl Com+*. 1981;17(10):996–998. doi: [10.1007/BF00503526](#)
- [13] Demus D, Zashcke H. Synthesis and properties of new liquid crystalline materials. *Mol Cryst Liq Cryst*. 1981;63(1):129–144. doi: [10.1080/00268948108071990](#)
- [14] Wolff R, Weissflog W, Kresse H, et al. Neue kristallin-flüssige ester mit einer dieyanethenyl-flügelgruppe. *Z Chem*. 1981;21(1):33–34. doi: [10.1002/zfch.19810210117](#)
- [15] Mikhaleva MA, Lazareva VT, Grebenkin MF, et al. Synthesis of Schiff bases of 2-substituted 5-aminopyrimidines and their mesomorphic properties. *Chem Heterocycl Com+*. 1982;18(11):1201–1208. doi: [10.1007/BF00506375](#)
- [16] Raines RD, Heffner WR, Cladis PE, et al. The dielectric constant of a cy anophenyl-thiobenzoate. *Mol Cryst Liq Cryst*. 1982;72(9–10):263–269. doi: [10.1080/01406568208084719](#)
- [17] Hong XJ, Ge MJ, Zhao XM, et al. Ortho cyano substituted negative dielectric anisotropic liquid crystals. *Mol Cryst Liq Cryst*. 1983;99(1):81–87. doi: [10.1080/00268948308072029](#)
- [18] Nakai H, Takenaka S, Kusabayashi S. Thermal and dielectric properties of liquid crystals with a coumarin skeleton. *B Chem Soc Jpn*. 1983;56(12):3571–3577. doi: [10.1246/bcsj.56.3571](#)
- [19] Osman MA, Huynh-Ba T. Nematogens for matrix-addressed twisted nematic displays - I. *Mol Cryst Liq Cryst*. 1983;82(10):331–338. doi: [10.1080/01406568308247027](#)
- [20] Takatsu H, Takeuchi K, Satō H. Synthesis and some physical properties of 1-cyclohexyl-2-(4"-halobiphenyl-4'-yl)ethanes. *Mol Cryst Liq Cryst*. 1983;100(3–4):345–355. doi: [10.1080/00268948308075363](#)
- [21] Kelly SM, Schad H. Some novel nematic liquid crystals of negative dielectric anisotropy. *Mol Cryst Liq Cryst*. 1984;110(1–4):239–261. doi: [10.1080/00268948408074508](#)
- [22] Schad H, Kelly SM. A novel liquid crystal compound with very large dielectric constants. *J Chem Phys*. 1984;81(3):1514–1515. doi: [10.1063/1.447757](#)
- [23] Osman MA. Liquid crystals with large negative dielectric anisotropy, part V. *Helv Chim Acta*. 1985;68(3):606–609.
- [24] Buchecker R, Schadt M. Synthesis, physical properties and structural relationships of new, end-chain substituted nematic liquid crystals. *Mol Cryst Liq Cryst*. 1987;149(1):359–373. doi: [10.1080/00268948708082991](#)
- [25] Reiffenrath V, Krause J, Plach HJ, et al. New liquid-crystalline compounds with negative dielectric anisotropy. *Liq Cryst*. 1989;5(1):159–170. doi: [10.1080/02678298908026359](#)
- [26] Schäfer W, Rosenfeld U, Zashcke H, et al. Kristallin-flüssige 1,3,4-thiadiazole. II [1]. 1,3,4-thiadiazole mit cyclohexanstrukturfragmenten. *J Prakt Chem*. 1989;331(4):631–636. doi: [10.1002/prac.19893310413](#)
- [27] Bartmann E, Dorsch D, Finkenzeller U. Liquid crystals with polar substituents containing fluorine: synthesis and physical properties. *Mol Cryst Liq Cryst*. 1991;204(1):77–89. doi: [10.1080/00268949108046596](#)
- [28] Pavluchenko AI, Smirnova NI, Petrov VF, et al. Synthesis and properties of liquid crystals with fluorinated terminal substituents. *Mol Cryst Liq Cryst*. 1991;209(1):225–235. doi: [10.1080/00268949108036197](#)
- [29] Bartmann E. Flüssigkristalle mit fluorhaltigen alkylgruppen. *Ber der Bunsengesellschaft für Physikalische Chem*. 1993;97(10):1349–1354. doi: [10.1002/bbpc.19930971027](#)
- [30] Reiffenrath V, Bremer M. Neue materialien für flüssigkristallanzeigen: struktur-eigenschafts-beziehungen bei 2-fluorpyridinen. *Angew Chem*. 1994;106(13):1435–1438. doi: [10.1002/ange.19941061318](#)
- [31] Beganskienė A, Adomėms P, Sirutkaitis R, et al. Synthesis and mesomorphic properties of 1,2-(4-substituted phenyl) ethynes containing fluoro atoms. *Mol Cryst Liq Cryst Sci Technol*. 1995;260(1):273–276. doi: [10.1080/10587259508038700](#)
- [32] Bremer M. Liquid crystals based on 2- fluoropyrimidine and -pyridine: synthesis, dielectric anisotropy and phase behavior*. *Adv Mater*. 1995;7(9):803–807.
- [33] Bremer M. Liquid crystals based on 2-fluoropyrimidine and -pyridine: synthesis, dielectric anisotropy and phase behavior*. *Adv Mater*. 1995;7(10):867–870.
- [34] Buchecker R, Marck G, Schadt M. New nematics incorporating a 2,6-difluorophenyl acetylene group. *Mol Cryst Liq Cryst Sci Technol*. 1995;260(1):93–105. doi: [10.1080/10587259508038685](#)
- [35] Demus D, Goto Y, Sawada S, et al. Trifluorinated liquid crystals for TFT displays. *Mol Cryst Liq Cryst Sci Technol*. 1995;260(1):1–21. doi: [10.1080/10587259508038680](#)
- [36] Goulding M, Greenfield S, Parri O, et al. Liquid crystals with a thiomethyl end group: lateral fluoro substituted 4-(trans-4-(n-propyl) cyclohexylethyl-4'-thiomethylbiphenyls and 4-n-alkyl-4"-thiomethylterphenyls. *Mol Cryst Liq Cryst Sci Technol*. 1995;265(1):27–40. doi: [10.1080/10587259508041675](#)
- [37] Greenfield S, Coates D, Goulding M, et al. Nematogenic laterally fluorinated biphenyls with polar terminal groups. *Liq Cryst*. 1995;18(4):665–672. doi: [10.1080/02678299508036672](#)
- [38] Karamysheva LA, Torgova SI, Agafonova IF, et al. Dependence of mesomorphic properties of 3,5-disubstituted 1,2,4-oxadiazoles on geometric and electronic factors. *Mol Cryst Liq Cryst Sci Technol*. 1995;260(1):217–225. doi: [10.1080/10587259508038693](#)
- [39] Pavluchenko AI, Smirnova NI, Petrov VF, et al. Synthesis and properties of new halogenated liquid

- crystals. *Mol Cryst Liq Cryst Sci Technol.* **1995**;265(1):41–45. doi: [10.1080/10587259508041676](https://doi.org/10.1080/10587259508041676)
- [40] Petrov VF, Pavluchenko AI, Smirnova NI. New liquid crystalline pyridine derivatives. *Mol Cryst Liq Cryst Sci Technol.* **1995**;265(1):47–53. doi: [10.1080/10587259508041677](https://doi.org/10.1080/10587259508041677)
- [41] Schmidt W, Vögtle F, Poetsch E. Spiro units as building blocks in thermotropic liquid crystals: synthesis and physical properties of terminally substituted spiro[5.5]undecanes. *Liebigs Annalen.* **1995**;1995(7):1319–1326.
- [42] Seils F, Schadt M. Liquid crystals with a chlorovinyl side chain; effect of structural variations on the dielectric anisotropy. *Mol Cryst Liq Cryst Sci Technol.* **1995**;260(1):127–138. doi: [10.1080/10587259508038687](https://doi.org/10.1080/10587259508038687)
- [43] Bartmann E. Liquid crystalline α , α -difluorobenzyl phenyl ethers. *Adv Mater.* **1996**;8(7):570–573. doi: [10.1002/adma.19960080707](https://doi.org/10.1002/adma.19960080707)
- [44] Kirsch P, Poetsch E. Novel polar liquid crystals with very low birefringence based on trans-1,3-dioxane building blocks. *Adv Mater.* **1998**;10(8):602–606. doi: [10.1002/\(SICI\)1521-4095\(199805\)10:8<602::AID-ADMA602>3.0.CO;2-8](https://doi.org/10.1002/(SICI)1521-4095(199805)10:8<602::AID-ADMA602>3.0.CO;2-8)
- [45] Kirsch P. Design and synthesis of nematic liquid crystals with negative dielectric anisotropy. *Liq Cryst.* **1999**;26(3):449–452. doi: [10.1080/026782999205236](https://doi.org/10.1080/026782999205236)
- [46] Kirsch P, Reiffenrath V, Bremer M. Nematic liquid crystals with negative dielectric anisotropy: molecular design and synthesis. *Synlett.* **1999**;1999(4):389–396. doi: [10.1055/s-1999-2619](https://doi.org/10.1055/s-1999-2619)
- [47] Petrov VF, Torgova SI, Karamysheva LA, et al. The trans-1,4-cyclohexylene group as a structural fragment in liquid crystals. *Liq Cryst.* **1999**;26(8):1141–1162. doi: [10.1080/026782999204174](https://doi.org/10.1080/026782999204174)
- [48] Kanie K, Tanaka Y, Takehara S, et al. A facile transformation of terminal olefins to *vic*-difluoro olefins: electro-optical properties of liquid crystalline materials having a *vic*-difluoro olefinic moiety. *B Chem Soc Jpn.* **2000**;73(7):1633–1643. doi: [10.1246/bcsj.73.1633](https://doi.org/10.1246/bcsj.73.1633)
- [49] Kirsch P, Bremer M. Nematic liquid crystals for active matrix displays: molecular design and synthesis. *Angew Chem.* **2000**;39(23):4216–4235. doi: [10.1002/1521-3773\(20001201\)39:23<4216::AID-ANIE4216>3.0.CO;2-K](https://doi.org/10.1002/1521-3773(20001201)39:23<4216::AID-ANIE4216>3.0.CO;2-K)
- [50] Kirsch P, Bremer M, Heckmeier M, et al. Liquid crystals with pentafluorosulfuranyl as a polar terminal group. *Mol Cryst Liq Cryst Sci Technol.* **2000**;346(1):29–33. doi: [10.1080/10587250008023862](https://doi.org/10.1080/10587250008023862)
- [51] Kirsch P, Bremer M, Kirsch A, et al. Materials for liquid crystal displays with reduced power consumption. *Mol Cryst Liq Cryst Sci Technol.* **2000**;346(1):193–199. doi: [10.1080/10587250008023878](https://doi.org/10.1080/10587250008023878)
- [52] Klasen M, Bremer M, Tarumi K. New liquid-crystal materials for active matrix displays with negative dielectric anisotropy and low rotational viscosity. *Jpn J Appl Phys.* **2000**;39(11B):L1180. doi: [10.1143/JJAP.39.L1180](https://doi.org/10.1143/JJAP.39.L1180)
- [53] Lim M, Kim SH, Lee YJ, et al. Physical properties of liquid crystal single compounds with 1,3,2-dioxaborinane group for LCD applications. *Mol Cryst Liq Cryst Sci Technol.* **2000**;352(1):319–326. doi: [10.1080/10587250008023189](https://doi.org/10.1080/10587250008023189)
- [54] Goulding M, Reiffenrath V, Hirschmann H. Highly birefringent nematic liquid crystals for reflective STN applications. *Mol Cryst Liq Cryst Sci Technol.* **2001**;364(1):899–910. doi: [10.1080/10587250108025063](https://doi.org/10.1080/10587250108025063)
- [55] Iwashita Y, Kaneoya M, Takeuchi K, et al. Physical property of new liquid crystal materials and mixture design for active matrix LCD. *Mol Cryst Liq Cryst Sci Technol.* **2001**;364(1):851–858. doi: [10.1080/10587250108025057](https://doi.org/10.1080/10587250108025057)
- [56] Kelly SM, O'Neill M. Liquid crystals, display and laser materials. In: Nalwa HS, editor. *Handbook of advanced electronic and photonic materials and devices*. Vol. 7. Elsevier; **2001**. p. 1–66. <https://booksite.elsevier.com/9780125137454/pdf/nal0701.pdf>
- [57] Kirsch P, Bremer M, Taugerbeck A, et al. Difluorooxymethylene-bridged liquid crystals: a novel synthesis based on the oxidative alkoxydifluorodesulfuration of dithianylum salts. *Angew Chem.* **2001**;40(8):1480–1484. doi: [10.1002/1521-3773\(20010417\)40:8<1480::AID-ANIE1480>3.0.CO;2-M](https://doi.org/10.1002/1521-3773(20010417)40:8<1480::AID-ANIE1480>3.0.CO;2-M)
- [58] Miyazawa K, Meijere AD. Liquid crystalline compounds with 2,2-disubstituted cyclopropane end groups in their side chains. *Mol Cryst Liq Cryst Sci Technol.* **2001**;364(1):529–546. doi: [10.1080/10587250108025023](https://doi.org/10.1080/10587250108025023)
- [59] Petrov VF, Shimizu Y. Isothiocyanato substitution in calamitic liquid crystals. *Mol Cryst Liq Cryst Sci Technol.* **2001**;363(1):107–121. doi: [10.1080/10587250108025262](https://doi.org/10.1080/10587250108025262)
- [60] Miyazawa K, Kato T, Itoh M, et al. First synthesis of liquid crystalline 2,3-bis(trifluoromethyl)phenyl derivatives exhibiting large negative dielectric anisotropy. *Liq Cryst.* **2002**;29(11):1483–1490. doi: [10.1080/02678290260372682](https://doi.org/10.1080/02678290260372682)
- [61] Miyazawa K, LÄhr S, De Meijere A. Liquid crystalline 2-cyclopropylcyclopropyl derivatives - synthesis and evaluation of the properties. *Mol Cryst Liq Cryst.* **2002**;373(1):83–103.
- [62] Petrov VF, Pavluchenko AI. Furan as a structural fragment in liquid crystals. *Mol Cryst Liq Cryst.* **2003**;393(1):1–13. doi: [10.1080/15421400390202881](https://doi.org/10.1080/15421400390202881)
- [63] Petrov VF, Pavluchenko AI. Nitrogen containing six-membered saturated heterocycles as structural fragments in liquid crystals. *Mol Cryst Liq Cryst.* **2003**;393(1):15–29. doi: [10.1080/15421400390202890](https://doi.org/10.1080/15421400390202890)
- [64] Sasada Y, Miyazawa K, Demus D. Liquid crystalline *N*-substituted-3,4-difluoropyrroles exhibiting large positive dielectric anisotropy. *Liq Cryst.* **2003**;30(12):1371–1375. doi: [10.1080/02678290310001628546](https://doi.org/10.1080/02678290310001628546)
- [65] Sun G-X, Chen B, Tang H, et al. Synthesis and physical properties of novel liquid crystals containing 2,3-difluorophenyl and 1,3-dioxane units. *J Mater Chem.* **2003**;13(4):742–748. doi: [10.1039/b210765a](https://doi.org/10.1039/b210765a)
- [66] Francis M, Ionescu D, Goulding M, et al. Improved liquid crystal mixtures for STN displays. *Mol Cryst Liq Cryst.* **2004**;411(1):71–78. doi: [10.1080/15421400490434801](https://doi.org/10.1080/15421400490434801)
- [67] Iwashita Y, Umezū Y, Kawakami S, et al. Liquid crystal mixtures with low birefringence for active-matrix LCD. *Mol Cryst Liq Cryst.* **2004**;411(1):41–48. doi: [10.1080/15421400490434559](https://doi.org/10.1080/15421400490434559)
- [68] Matsui S, Kondo T, Sago K. Synthesis and properties of novel liquid crystalline compounds having a difluoromethyleneoxy moiety as a linkage group. *Mol Cryst Liq Cryst.* **2004**;411(1):127–137. doi: [10.1080/15421400490434919](https://doi.org/10.1080/15421400490434919)

- [69] Bremer M, Lietzau L. 1,1,6,7-tetrafluoroindanes: improved liquid crystals for LCD-TV application. *New J Chem.* **2005**;29(1):72. doi: [10.1039/b414312d](https://doi.org/10.1039/b414312d)
- [70] Keum H-W, Roh S-D, Do YS, et al. Synthesis and physical properties of novel fluorinated liquid crystalline compounds. *Mol Cryst Liq Cryst.* **2005**;439(1):[189]/[2055]–[199]/[2065]. doi: [10.1080/15421400590955352](https://doi.org/10.1080/15421400590955352)
- [71] Bremer M, Klasen-Memmer M, Pauluth D, et al. Novel liquid-crystal materials with negative dielectric anisotropy for TV application. *J Soc Inf Disp.* **2006**;14(6):517–521. doi: [10.1889/1.2210801](https://doi.org/10.1889/1.2210801)
- [72] Januszko A, Glab KL, Kaszynski P, et al. The effect of carborane, bicyclo[2.2.2]octane and benzene on mesogenic and dielectric properties of laterally fluorinated three-ring mesogens. *J Mater Chem.* **2006**;16(31):3183. doi: [10.1039/b600068a](https://doi.org/10.1039/b600068a)
- [73] Kirsch P, Binder JT, Lork E, et al. Liquid crystals based on hypervalent sulfur fluorides. *J Fluorine Chem.* **2006**;127(4–5):610–619. doi: [10.1016/j.jfluchem.2005.11.015](https://doi.org/10.1016/j.jfluchem.2005.11.015)
- [74] Kirsch P, Hahn A, Fröhlich R, et al. Liquid crystals based on axially fluorinated 1,3-dioxanes: synthesis, properties and computational study. *Eur J Org Chem.* **2006**;2006(21):4819–4824. doi: [10.1002/ejoc.200600529](https://doi.org/10.1002/ejoc.200600529)
- [75] Kirsch P, Maillard D. A convenient synthetic route to tetrahydropyran-Based liquid crystals. *Eur J Org Chem.* **2006**;2006(15):3326–3331. doi: [10.1002/ejoc.200600160](https://doi.org/10.1002/ejoc.200600160)
- [76] Hird M. Fluorinated liquid crystals – properties and applications. *Chem Soc Rev.* **2007**;36(12):2070.
- [77] Kirsch P, Lenges M, Ruhl A, et al. Liquid crystals with partially fluorinated side chains: highly polar materials with very low birefringence. *J Fluorine Chem.* **2007**;128(10):1221–1226. doi: [10.1016/j.jfluchem.2007.04.010](https://doi.org/10.1016/j.jfluchem.2007.04.010)
- [78] Sago K, Fujita A. Synthesis and properties of novel liquid crystalline compounds having fluorinated ring systems. *Mol Cryst Liq Cryst.* **2007**;479(1):[151]/[1189]–[160]/[1198]. doi: [10.1080/15421400701732555](https://doi.org/10.1080/15421400701732555)
- [79] Sasada Y, Shimada T, Ushioda M, et al. Synthesis and properties of novel 1,1-difluoropropoxy-linked liquid crystalline compounds of negative dielectric anisotropy. *Liq Cryst.* **2007**;34(5):569–576. doi: [10.1080/02678290701284279](https://doi.org/10.1080/02678290701284279)
- [80] Xianyu H, Gauza S, Song Q, et al. High birefringence and large negative dielectric anisotropy phenyl-tolane liquid crystals. *Liq Cryst.* **2007**;34(12):1473–1478. doi: [10.1080/02678290701730065](https://doi.org/10.1080/02678290701730065)
- [81] Goto M, Masukawa T, Kondo T, et al. Novel nematic liquid crystalline compounds having a tetrahydropyran ring. *Mol Cryst Liq Cryst.* **2008**;494(1):58–67. doi: [10.1080/15421400802430042](https://doi.org/10.1080/15421400802430042)
- [82] Kirsch P, Binder W, Hahn A, et al. Super-fluorinated liquid crystals: towards the limits of polarity. *Eur J Org Chem.* **2008**;2008(20):3479–3487. doi: [10.1002/ejoc.200800149](https://doi.org/10.1002/ejoc.200800149)
- [83] Yokokoji O, Shimizu K, Inoue S. 5,6-difluoro-1h-indene derivatives: novel core structure of liquid crystals with high Δn and $\Delta\epsilon$. *Liq Cryst.* **2009**;36(1):1–6. doi: [10.1080/02678290802680813](https://doi.org/10.1080/02678290802680813)
- [84] Dąbrowski R, Dziaduszek J, Garbat K, et al. Synthesis and mesogenic properties of three- and four-ring compounds with a fluoroisothiocyanatobiphenyl moiety. *Liq Cryst.* **2010**;37(12):1529–1537. doi: [10.1080/02678292.2010.521983](https://doi.org/10.1080/02678292.2010.521983)
- [85] Kirsch P, Bremer M. Understanding fluorine effects in liquid crystals. *Chemphyschem.* **2010**;11(2):357–360. doi: [10.1002/cphc.200900745](https://doi.org/10.1002/cphc.200900745)
- [86] Petrov VF. Cyclopentane as a structural fragment in liquid crystals. *Mol Cryst Liq Cryst.* **2010**;517(1):10–26. doi: [10.1080/15421400903507755](https://doi.org/10.1080/15421400903507755)
- [87] Urban S, Kula P, Spadło A, et al. Dielectric properties of selected laterally fluoro-substituted 4,4'-dialkyl, dialkoxy and alkyl-alkoxy [1: 1';4': 1'']terphenyls. *Liq Cryst.* **2010**;37(10):1321–1330. doi: [10.1080/02678292.2010.505665](https://doi.org/10.1080/02678292.2010.505665)
- [88] Dziaduszek J, Kula P, Dąbrowski R, et al. General synthesis method of alkyl-alkoxy multi-fluorotolanes for negative high birefringence nematic mixtures. *Liq Cryst.* **2012**;39(2):239–247. doi: [10.1080/02678292.2011.636457](https://doi.org/10.1080/02678292.2011.636457)
- [89] Ponomarenko MV, Kalinovich N, Serguchev YA, et al. Synthesis of pentafluoro- λ 6-sulfanyl substituted acetylenes for novel liquid crystals. *J Fluorine Chem.* **2012**;135:68–74. doi: [10.1016/j.jfluchem.2011.08.011](https://doi.org/10.1016/j.jfluchem.2011.08.011)
- [90] Bremer M, Kirsch P, Klasen-Memmer M, et al. The TV in your pocket: development of liquid-crystal materials for the new millennium. *Angew Chem.* **2013**;52(34):8880–8896. doi: [10.1002/anie.201300903](https://doi.org/10.1002/anie.201300903)
- [91] Jankowiak A, Ringstrand B, Januszko A, et al. Liquid crystals with negative dielectric anisotropy: the effect of unsaturation in the terminal chain on thermal and electro-optical properties. *Liq Cryst.* **2013**;40(5):605–615. doi: [10.1080/02678292.2013.774064](https://doi.org/10.1080/02678292.2013.774064)
- [92] Kula P, Aptacy A, Herman J, et al. The synthesis and properties of fluoro-substituted analogues of 4-butyl-4'-[(4-butylphenyl)ethynyl]biphenyls. *Liq Cryst.* **2013**;40(4):482–491. doi: [10.1080/02678292.2012.757813](https://doi.org/10.1080/02678292.2012.757813)
- [93] Al-Maharik N, Kirsch P, Slawin AMZ, et al. The influence of vicinal threo-difluorination on electro-optic and mesogenic properties of propyleneoxy-linked nematic liquid crystals. *Tetrahedron.* **2014**;70(31):4626–4630. doi: [10.1016/j.tet.2014.05.027](https://doi.org/10.1016/j.tet.2014.05.027)
- [94] Araki K, Yamamoto T, Tanaka R, et al. Stereoselective synthesis and physicochemical properties of liquid-crystal compounds possessing a *trans*-2,5-disubstituted tetrahydropyran ring with negative dielectric anisotropy. *Chem – Eur J.* **2014**;21(6):2458–2466.
- [95] Gotoh Y, Ushioda M. Synthesis and physicochemical properties of novel liquid crystal compounds with negative dielectric anisotropy with a tetrahydropyran ring: part 2. *Mol Cryst Liq Cryst.* **2014**;593(1):61–77. doi: [10.1080/15421406.2013.867224](https://doi.org/10.1080/15421406.2013.867224)
- [96] Kirsch P, Bremer M. Hypervalent sulfur fluorides and the design of liquid crystals. *Chimia (Aarau).* **2014**;68(6):363. doi: [10.2533/chimia.2014.363](https://doi.org/10.2533/chimia.2014.363)
- [97] Lee T-H, Chen J-T, Hsu C-S. Synthesis of cyclopentyl-oxo terphenyl liquid crystals with negative dielectric anisotropy. *Liq Cryst.* **2014**;42(1):104–112.
- [98] Hu M, Li J, Li J, et al. Synthesis and properties of difluoromethyleneoxy-bridged liquid crystals terminated by 2,2-difluorovinyl-oxo group. *Liq Cryst.* **2015**;42(3):383–389. doi: [10.1080/02678292.2014.992375](https://doi.org/10.1080/02678292.2014.992375)

- [99] Kirsch P. Fluorine in liquid crystal design for display applications. *J Fluorine Chem.* **2015**;177:29–36. doi: [10.1016/j.jfluchem.2015.01.007](https://doi.org/10.1016/j.jfluchem.2015.01.007)
- [100] Li F, An Z, Chen X, et al. Synthesis and the effect of 2,3-difluoro substitution on the properties of diarylacetylene terminated by an allyloxy group. *Liq Cryst.* **2015**;42(11):1654–1663. doi: [10.1080/02678292.2015.1084657](https://doi.org/10.1080/02678292.2015.1084657)
- [101] Li J, Yang X, Gan N, et al. The effect of lateral fluorination on the properties of phenyl-tolane liquid crystals. *Liq Cryst.* **2015**;42(3):397–403. doi: [10.1080/02678292.2014.995241](https://doi.org/10.1080/02678292.2014.995241)
- [102] Szczuciński Ł, Dąbrowski R, Urban S, et al. Synthesis, mesogenic and dielectric properties of fluorosubstituted isothiocyanatoterphenyls. *Liq Cryst.* **2015**;42(12):1706–1729. doi: [10.1080/02678292.2015.1070924](https://doi.org/10.1080/02678292.2015.1070924)
- [103] Al-Maharik N, Kirsch P, Slawin AMZ, et al. Fluorinated liquid crystals: evaluation of selectively fluorinated facially polarised cyclohexyl motifs for liquid crystal applications. *Org Biomol Chem.* **2016**;14(42):9974–9980. doi: [10.1039/C6OB01986B](https://doi.org/10.1039/C6OB01986B)
- [104] Kirsch P. Fluorinated nematic liquid crystals. In: Tressaud A, Poeppelmeier K, editors. *Photonic and electronic properties of fluoride materials*. Elsevier; **2016**. p. 159–176. <https://www.sciencedirect.com/science/chapter/edited-volume/abs/pii/B9780128016398000088>
- [105] Chen R, Zhao L, An Z, et al. Synthesis and properties of allyloxy-based tolane liquid crystals with high negative dielectric anisotropy. *Liq Cryst.* **2017**;44(14–15):2184–2191. doi: [10.1080/02678292.2017.1360525](https://doi.org/10.1080/02678292.2017.1360525)
- [106] Song K, Li J, Li J, et al. New terphenyl liquid crystals terminated by 2-chloro-3,3,3-trifluoropropenyl group. *Liq Cryst.* **2017**;44(11):1646–1652. doi: [10.1080/02678292.2017.1306634](https://doi.org/10.1080/02678292.2017.1306634)
- [107] Yamada S, Hashishita S, Asai T, et al. Design, synthesis and evaluation of new fluorinated liquid crystals bearing a CF₂CF₂ fragment with negative dielectric anisotropy. *Org Biomol Chem.* **2017**;15(6):1495–1509. doi: [10.1039/C6OB02431A](https://doi.org/10.1039/C6OB02431A)
- [108] Yamada S, Hashishita S, Konishi H, et al. New entry for fluorinated carbocycles: unprecedented 3,6-disubstituted 1,1,2,2-tetrafluorocyclohexane derivatives. *J Fluorine Chem.* **2017**;200:47–58. doi: [10.1016/j.jfluchem.2017.05.013](https://doi.org/10.1016/j.jfluchem.2017.05.013)
- [109] Yamada S, Tamamoto K, Kida T, et al. Rational design and synthesis of a novel laterally-tetrafluorinated tricyclic mesogen with large negative dielectric anisotropy. *Org Biomol Chem.* **2017**;15(44):9442–9454. doi: [10.1039/C7OB02399E](https://doi.org/10.1039/C7OB02399E)
- [110] Dai Y, Gao L, Chang Y, et al. Dielectric and elastic properties of fluorine-containing tricyclic isothiocyanate liquid crystal. *Liq Cryst.* **2018**;46(6):930–940.
- [111] Herman J, Harmata P, Strzeżysz O, et al. Synthesis and properties of chosen 4-butyl-phenyltolane derivatives – on the influence of core substitution on birefringence, mesomorphic and dielectric properties. *J Mol Liq.* **2018**;267:511–519. doi: [10.1016/j.molliq.2017.04.090](https://doi.org/10.1016/j.molliq.2017.04.090)
- [112] Fang Z, Al-Maharik N, Kirsch P, et al. Synthesis of organic liquid crystals containing selectively fluorinated cyclopropanes. *Beilstein J Org Chem.* **2020**;16:674–680. doi: [10.3762/bjoc.16.65](https://doi.org/10.3762/bjoc.16.65)
- [113] Hu K, Weng Q, Chen R, et al. Benzoxazole-terminated liquid crystals with high birefringence and large dielectric anisotropy. *Liq Cryst.* **2020**;47(9):1274–1280. doi: [10.1080/02678292.2019.1710777](https://doi.org/10.1080/02678292.2019.1710777)
- [114] Li J, Che Z, Mo L, et al. 5,6-difluorobenzofuran: a new core for the design of liquid crystal compound with large dielectric anisotropy and broad nematic range. *Liq Cryst.* **2020**;48(2):273–280.
- [115] Li J, Yang X, Wan D, et al. Increasing the negative dielectric anisotropy of liquid crystals by fluorination of the terminal ethyl chain. *Liq Cryst.* **2020**;47(14–15):2268–2275. doi: [10.1080/02678292.2020.1769755](https://doi.org/10.1080/02678292.2020.1769755)
- [116] Mo L, Li J, Che Z, et al. New negative dielectric anisotropy liquid crystals based on benzofuran core. *Liq Cryst.* **2020**;47(14–15):2313–2322. doi: [10.1080/02678292.2020.1795946](https://doi.org/10.1080/02678292.2020.1795946)
- [117] Wan D, Gu X, Li J, et al. Synthesis and properties of isothiocyanate liquid crystals containing cyclohexene unit. *Liq Cryst.* **2021**;48(10):1392–1401. doi: [10.1080/02678292.2021.1873436](https://doi.org/10.1080/02678292.2021.1873436)
- [118] Wan D, Shi F, Che Z, et al. Introduction of 5,6-dihydro-4H-cyclopenta[b]thiophene core unit into phenyltolane: expanding the mesophase range and increasing the birefringence and dielectric anisotropy of liquid crystal. *Liq Cryst.* **2021**;48(12):1650–1659. doi: [10.1080/02678292.2021.1897892](https://doi.org/10.1080/02678292.2021.1897892)
- [119] Wan D, Yang X, Li J, et al. Synthesis and properties of 5,6-dihydro-4H-cyclopenta[b]thiophene-based nematic liquid crystals: a new access to mesogens with high birefringence and large dielectric anisotropy. *J Mol Liq.* **2021**;327:114827. doi: [10.1016/j.molliq.2020.114827](https://doi.org/10.1016/j.molliq.2020.114827)
- [120] Li J, Mo L, Che Z, et al. New multi-fluorinated benzofuran liquid crystals with large dielectric anisotropy and improved solubility. *Liq Cryst.* **2022**;49(13):1753–1762. doi: [10.1080/02678292.2022.2061057](https://doi.org/10.1080/02678292.2022.2061057)
- [121] Wan D, Che Z, Mo L, et al. Synthesis and properties of fluorinated terphenyl liquid crystals utilizing 5,6-dihydro-4H-cyclopenta[b]thiophene as core unit. *J Mol Struct.* **2022**;1267:133612. doi: [10.1016/j.molstruc.2022.133612](https://doi.org/10.1016/j.molstruc.2022.133612)
- [122] Qian Y, Li S, Tang H, et al. Effect of substituents on the properties of fluorine-containing polyphenyl liquid crystal compounds. *J Mol Liq.* **2023**;391:123289. doi: [10.1016/j.molliq.2023.123289](https://doi.org/10.1016/j.molliq.2023.123289)
- [123] Tang J, Yao C, An Z, et al. Balance the trade-offs between high birefringence, large dielectric anisotropy and low viscosity in nematic liquid crystals through molecular splicing strategy. *Liq Cryst.* **2023**;50(11–12):1902–1910. doi: [10.1080/02678292.2023.2222677](https://doi.org/10.1080/02678292.2023.2222677)
- [124] Zhang T, Liang F, Li X, et al. Novel benzoxazole-based liquid crystals with negative dielectric anisotropy and moderate optical anisotropy. *Liq Cryst.* **2023**;50(15):2446–2457. doi: [10.1080/02678292.2023.2259843](https://doi.org/10.1080/02678292.2023.2259843)
- [125] Zhang T, Liang F, Lin H, et al. Benzoxazole-terminated liquid crystals with large birefringence and negative dielectric anisotropy. *J Mol Liq.* **2023**;389:122859.
- [126] Mo L, Wan D, Li J, et al. Synthesis and properties of dibenzofuran- and dibenzothiophene-based mesogens: an effective access to liquid crystals with large negative dielectric anisotropy. *J Mol Liq.* **2024**;405:125061. doi: [10.1016/j.molliq.2024.125061](https://doi.org/10.1016/j.molliq.2024.125061)

- [127] Wan D, Mo L, Che Z, et al. Utilizing bicyclohexene as a building block: a promising approach to achieve negative liquid crystals with lower melting points. *J Mol Struct.* **2025**;1322:140542. doi: [10.1016/j.molstruc.2024.140542](https://doi.org/10.1016/j.molstruc.2024.140542)
- [128] Davis EJ, Mandle RJ, Russell BK, et al. Liquid-crystalline structure-property relationships in halogen-terminated derivatives of cyanobiphenyl. *Liq Cryst.* **2014**;41(11):1635–1646.
- [129] Mandle RJ, Goodby JW. An interplay between molecular pairing, smectic layer spacing, dielectric anisotropy and re-entrant phenomena in -alkenyloxy cyanobiphenyls. *Liq Cryst.* **2017**;44(4):656–665.
- [130] Bremer M, Reiffenrath V, Pauluth D, et al. Inventors; Merck Patent GmbH, assignee. 3,4,5-trifluorophenyl 4-cyclohexylbenzoates. US patent US 5725799 A. **1998** [1996 Nov 1].
- [131] Bremer M, Tarumi K, Krause J. Inventors; Merck Patent GmbH, assignee. Fluorinated biphenylcyclohexanes, and liquid-crystalline medium. US patent US 5807500 A. **1998** [1996 Apr 29].
- [132] Haseba Y, Matsui S, Miyazawa K, et al. Inventors; Chisso Corp, assignee. Dioxane derivative having fluoroalkyl group, liquid crystal composition and liquid crystal display element. JP patent JP H10139778 A. **1998** [1996 Nov 7].
- [133] Kobayashi K, Matsui S, Miyazawa K, et al. Inventors; Chisso Corp, assignee. Halogen-substituted benzene derivative, liquid crystal composition and liquid crystal element. JP patent JP H10251186 A. **1998** [1997 Mar 10].
- [134] Matsui S, Kondo T, Haseba Y, et al. Inventors; Chisso Corp, assignee. Novel trifluorophenyl derivative. JP patent JP H10316969 A. **1998** [1997 May 16].
- [135] Matsui S, Takeuchi H, Miyazawa K. Inventors; Chisso Corp, assignee. Thion-o-ester derivative and its production. JP patent JP H1017544 A. **1998** [1996 Jul 2].
- [136] Miyazawa K, Yano H. Inventors; Chisso Corp, assignee. Liquid crystalline compound having negative anisotropic value of dielectric constant, liquid crystal composition containing the same liquid crystalline compound and liquid crystal display element using the same liquid crystal composition. JP patent JP H10237075 A. **1998** [1997 Feb 24].
- [137] Yamada K, Yano H. Inventors; Chisso Corp, assignee. Liquid-crystalline compound having negative dielectric anisotropy value, liquid crystal composition containing the liquid-crystalline compound, and liquid crystal display element using the liquid crystal composition. JP patent JP H10237035 A. **1998** [1997 Feb 26].
- [138] Yamada K, Yano H. Inventors; Chisso Corp, assignee. Liquid crystalline compound with negative permittivity anisotropy, liquid crystal composition containing the same, and liquid crystal element prepared from the composition. JP patent JP H10237448 A. **1998** [1997 Feb 26].
- [139] Yamada K, Yano H. Inventors; Chisso Corp, assignee. Liquid crystal compound having negative anisotropic value of dielectric constant, liquid crystal composition containing the same and liquid crystal display element using the composition. JP patent JP H10236993 A. **1998** [1997 Feb 26].
- [140] Yano H, Matsui S, Takeuchi H, et al. Inventors; Chisso Corp, assignee. Liquid crystal compound having negative permittivity anisotropic value, liquid crystal composition containing the liquid crystal compound and liquid crystal display element using the composition. JP patent JP H10168076 A. **1998** [1997 Feb 20].
- [141] Yano H, Takeuchi H. Inventors; Chisso Corp, assignee. Liquid crystal compound having negative anisotropy in permittivity, liquid crystal composition containing this compound, and liquid crystal display element made by using this composition. JP patent JP H10168453 A. **1998** [1997 Feb 20].
- [142] Andou T, Shibata K, Matsui S, et al. Inventors; Chisso Corp, assignee. Polyhaloalkyl ether derivatives as well as liquid crystal compositions and liquid crystal display elements containing them. US patent US 6007740 A. **1999** [1997 Nov 7].
- [143] Kirsch P, Tarumi K, Krause J. Inventors; Merck Patent GmbH, assignee. Halovinyl-oxy-substituted dioxane derivatives. US patent US 5997766 A. **1999** [1997 Dec 24].
- [144] Kirsch P, Tarumi K, Krause J. Inventors; Merck Patent GmbH, assignee. 1,3-dioxane derivatives having axial fluorine substitution. US patent US 5961880 A. **1999** [1998 Jun 4].
- [145] Miyazawa K, Matsui S, Takeuchi H, et al. Inventors; Chisso Corp, assignee. Liquid crystalline compound having alkynyl group, and liquid crystal compositions and liquid crystal display device therefrom. US patent US 5879585 A. **1999** [1997 Oct 10].
- [146] Bernhard H, Kresse H, Demus D, et al. Inventors; Chisso Corp, assignee. Liquid-crystal compounds having large value of permittivity anisotropy, liquid-crystal composition containing the same, and liquid-crystal display element made using the liquid-crystal composition. EP patent EP 1010692 A1. **2000** [1998 Jul 3].
- [147] Fujita A, Tamura N, Matsui S, et al. Inventors; Chisso Corp, assignee. Conjugated nitrile derivative, liquid crystal composition, and liquid crystal display elements. US patent US 6149838 A. **2000** [1999 May 28].
- [148] Inagaki J, Harufuji T, Koizumi Y, et al. Inventors; Chisso Corp, assignee. Thioether compound, liquid crystal composition and liquid crystal display element having negative value of permittivity anisotropy. JP patent JP 2000256307 A. **2000** [1999 Mar 9].
- [149] Kirsch P, Tarumi K, Krause J. Inventors; Merck Patent GmbH, assignee. Cyclohexane derivatives, and liquid-crystalline medium. US patent US 6139773 A. **2000** [1998 Jun 4].
- [150] Kirsch P, Tarumi K, Krause J, et al. Inventors; Merck Patent GmbH, assignee. Fluorocyclohexane derivatives, and liquid-crystalline medium. US patent US 6056895 A. **2000** [1998 Apr 7].
- [151] Kondo T, Matsui S, Miyazawa K, et al. Inventors; Chisso Corp, assignee. Fluoro-substituted alkyl ether compounds, liquid crystal compositions and liquid crystal display devices. US patent US 6124005 A. **2000** [1998 Dec 14].

- [152] Miyazawa K, Takeuchi H, Yagi Y, et al. Inventors; Chisso Corp, assignee. 2,3-difluorophenyl derivatives having negative value of permittivity anisotropy, liquid-crystal composition, and liquid-crystal display element. EP patent EP 1026142 A1. [2000](#) [1998 Oct 26].
- [153] Miyazawa K, Takeuchi H, Yano H. Inventors; Chisso Corp, assignee. Liquid crystal compound having negative dielectric anisotropy, liquid crystal composition containing said liquid crystal compound and liquid crystal display device using said composition. EP patent EP 0982386 A1. [2000](#) [1998 Aug 21].
- [154] Miyazawa K, Yano H. Inventors; Chisso Corp, assignee. Liquid crystal compound having negative dielectric anisotropy, liquid crystal composition containing said liquid crystal compound and liquid crystal display device using said composition. EP patent EP 0982388 A1. [2000](#) [1998 Aug 24].
- [155] Yamada K, Yano H, Inventors; Chisso Corp, assignee. Liquid crystal compound having negative dielectric anisotropy, liquid crystal composition containing said liquid crystal compound and liquid crystal display device using said composition. EP patent EP 0982387 A1. [2000](#) [1998 Aug 24].
- [156] Andou T, Matsui S, Miyazawa K, et al. Inventors; Chisso Corp, assignee. Liquid crystalline compound, liquid crystal composition comprising the liquid crystalline compound, and liquid crystal display device using the liquid crystal composition. US patent US 6319570 B1. [2001](#) [2000 Jun 19].
- [157] Chandler Clive D. Inventor; FEI Co, assignee. Method and apparatus for selective in-situ etching of inter dielectric layers. US patent US 6268608 B1. [2001](#) [1998 Oct 9].
- [158] Haseba Y, Miyazawa K, Matsui S, et al. Inventors; Chisso Corp, assignee. Liquid-crystal compounds having fluorinated alkyl groups, liquid-crystal composition, and liquid-crystal display element. US patent US 6248260 B1. [2001](#) [1999 Jul 28].
- [159] Kato T, Miyazawa K, Matsui S, et al. Inventors; Chisso Corp, assignee. Compound having alkadienyl group as side chain, and liquid crystal composition using same. US patent US 6174457 B1. [2001](#) [1999 Feb 11].
- [160] Koga K, Ando T, Takeuchi H, et al. Inventors; Chisso Corp, assignee. Tetracyclic compound having lateral halogen substituent and liquid crystal composition comprising the same. US patent US 6174458 B1. [2001](#) [1999 Feb 26].
- [161] Takatsu H, Saito Y, Frings Rainer B, et al. Inventors; Dainippon Ink & Chemicals, assignee. Compound having tetralhydronaphthalene skeleton and liquid crystal composition containing the same. CA patent CA 2377217 A1. [2001](#) [1999 Oct 10].
- [162] Tamura N, Fujita A, Matsui S, et al. Inventors; Chisso Corp, assignee. Liquid-crystal alkenyltolan derivative, liquid-crystal composition, and liquid-crystal display element. US patent US 6333080 B1. [2001](#) [1999 May 6].
- [163] Tamura N, Fujita A, Matsui S, et al. Inventors; Chisso Corp, assignee. Liquid crystalline compound having piperidine ring, liquid crystal composition and liquid crystal display element. EP patent EP 1072593 A1. [2001](#) [1999 Mar 30].
- [164] Bremer M, Pauluth D, Krause J, et al. Inventors; Merck GmbH, assignee. Fluorocyclohexene derivatives, and liquid-crystalline medium. US patent US 6475595 B1. [2002](#) [2000 Mar 31].
- [165] Kondo T, Matsui S, Miyazawa K, et al. Inventors; Chisso Corp, assignee. Vinylene compounds and liquid-crystal composition. US patent US 6337034 B1. [2002](#) [1998 Aug 24].
- [166] Kondo T, Sagou K, Matsui S, et al. Inventors; Chisso Corp, assignee. Difluoromethyl ether derivative and process for producing the same. EP patent EP 1182186 A2. [2002](#) [2001 Aug 10].
- [167] Miyazawa K, Takeuchi H, Kubo Y, et al. Inventors; Chisso Corp, assignee. Liquid-crystal compounds having large negative value of permittivity anisotropy, liquid-crystal composition, and liquid-crystal display element. US patent US 6348244 B1. [2002](#) [2000 Apr 24].
- [168] Tamura N, Takeuchi H, Matsui S, et al. Inventors; Chisso Corp, assignee. Fluoroalkoxybenzene derivatives having ether bond, liquid-crystal composition, and liquid-crystal display element. US patent US 6372153 B1. [2002](#) [2000 Mar 13].
- [169] Bremer M, Heckmeier M, Krause J, et al. Inventors; Merck Patent GmbH, assignee. Ester compounds and their use in liquid-crystalline media. US patent US 6541081 B1. [2003](#) [2000 Nov 15].
- [170] Bremer M, Kirsch P, Pauluth D, et al. Inventors; Merck Patent GmbH, assignee. Dioxane derivatives, and liquid-crystalline medium. US patent US 6620468 B2. [2003](#) [2001 Aug 6].
- [171] Kirsch P, Krause J, Luessem G, et al. Inventors; Merck Patent GmbH, assignee. Tetracyclic and pentacyclic compounds, and their use in liquid-crystalline media. US patent US 6635318 B2. [2003](#) [2001 Aug 13].
- [172] Kondou T, Matsui S, Miyazawa K, et al. Inventors; Chisso Corp, assignee. Terphenyl derivative, liquid crystal composition and liquid crystal display device. US patent US 6596349 B2. [2003](#) [2001 Apr 18].
- [173] Matsui S, Sasada Y, Miyazawa K, et al. Inventors; Chisso Corp, assignee. Liquid crystalline compound having difluoropropyleneoxy group as bonding group, liquid crystal composition and liquid crystal display element. JP patent JP 2003002858 A. [2003](#) [2001 Aug 10].
- [174] Rainer L, Kazhushkov S, De Meijere A, et al. Inventors; Chisso Corp, assignee. Bicyclo[3.1.0]hexane derivative. JP patent JP 2003261470 A. [2003](#) [2002 Mar 5].
- [175] Sasada Y, Demus D. Inventors; Chisso Corp, assignee. Liquid crystalline 3,4-substituted pyrrole. JP patent JP 2003277359 A. [2003](#) [2003 Jan 16].
- [176] Sasada Y, Miyazawa K, Kubo Y, et al. Inventors; Chisso Corp, assignee. Liquid crystal compound, liquid crystal composition and liquid crystal display element. JP patent JP 2003128665 A. [2003](#) [2002 Mar 29].
- [177] Sasada Y, Miyazawa K, Muraki K, et al. Inventors; Chisso Corp, assignee. Liquid crystal compound, liquid crystal composition and liquid crystal display element. JP patent JP 2003081967 A. [2003](#) [2001 Sep 13].
- [178] Tamura N, Fujita A, Takeuchi H, et al. Inventors; Chisso Corp, assignee. Liquid crystal compounds exhibiting negative anisotropy of permittivity. US patent US 6576303 B1. [2003](#) [2000 Aug 24].

- [179] Tokuyuki I, Shuichi M, Hiroyuki T, et al. Inventors; Chisso Corp, assignee. Liquid crystal compound containing unsaturated bond in bond group, liquid crystal composition and liquid crystal display element. JP patent, JP 3579756 B2. 2004 [1996 Jun 4].
- [180] Bremer M, Pauluth D, Heckmeier M, et al. Inventors; Merck Patent Beschraenkter Haf, assignee. Fluorinated (dihydro)phenanthrene derivatives, and their use in liquid-crystalline media. US patent US 6793984 B2. 2004 [2002 Jun 7].
- [181] Haseba Y, Matsui S, Takeuchi H, et al. Inventors; Chisso Corp, assignee. Ester compounds, liquid crystal compositions and liquid crystal display devices. US patent US 6685995 B1. 2004 [2000 Jul 7].
- [182] Kirsch P, Heckmeier M, Krause J, et al. Inventors; Merck Patent GmbH, assignee. Liquid-crystalline compounds. US patent US 6723866 B2. 2004 [2002 Jul 25].
- [183] Kirsch P, Huber F, Krause J, et al. Inventors; Merck Patent GmbH, assignee. Liquid-crystalline compounds. US patent US 6706338 B2. 2004 [2001 Dec 21].
- [184] Kirsch P, Pauluth D, Krause J, et al. Inventors; Merck Patent GmbH, assignee. Liquid crystalline compounds. US patent US 6780477 B2. 2004 [2003 Jun 12].
- [185] Matsui S, Koizumi Y, Miyazawa K, et al. Inventors; Chisso Corp, assignee. Liquid crystal compounds having fluorinated linkages, liquid crystal compositions, and liquid crystal display devices. EP patent EP 0893423 B1. 2004 [1997 Apr 9].
- [186] Sasada Y. Inventor; Chisso Corp, assignee. Compound containing bis(trifluoromethyl)vinyl group, liquid crystal composition and liquid crystal display element. JP patent JP 2004217552 A. 2004 [2003 Jan 14].
- [187] Sugiura M, Furuya M. Inventors; Chisso Corp, assignee. Propionate ester derivative, liquid crystal composition containing the derivative and liquid crystal display element containing the liquid crystal composition. JP patent JP 2004075667 A. 2004 [2003 Jun 4].
- [188] Kato T. Inventor; Chisso Corp, assignee. Compound having perfluoropropenyl, liquid crystal composition and liquid crystal display element. JP patent JP 2005298466 A. 2005 [2004 May 13].
- [189] Miyazawa K, Kato T, Kubo Y, et al. Inventors; Chisso Corp, assignee. Chisso Petrochemical Corp, assignee. Liquid crystal compounds having bis(trifluoromethyl) phenyl rings, liquid crystal compositions and liquid crystal display devices. US patent US 6844032 B2. 2005 [2002 Mar 29].
- [190] Sugiura M, Shioda M. Inventors; Chisso Corp, assignee. Chroman compound, liquid crystal composition containing the same and liquid crystal-displaying element containing the composition. JP patent JP 2005035986 A. 2005 [2004 Jun 22].
- [191] Bremer M, Klasen-Memmer M, Hornung B, et al. Inventors; Merck Patent GmbH, assignee. Fluorinated naphthalenes, liquid-crystal mixtures comprising them, and liquid-crystal displays. US patent US 7014890 B2. 2006 [2003 Jun 9].
- [192] Bremer M, Pauluth D, Klasen-Memmer M. Inventors; Merck Patent GmbH, assignee. Fluorinated fluorene derivatives. US patent US 7087272 B2. 2006 [2003 Sep 29].
- [193] Goulding Mark J, Duffy W, Adlem K, et al. Inventors; Merck Patent GmbH, assignee. Pyrans as liquid crystals. US patent US 7022865 B2. 2006 [2004 May 27].
- [194] Kang Jie D. Inventor; Shijiazhuang Yongsheng Huasing, assignee. Olefine compound, preparing method and use thereof. CN patent CN 1273428 C. 2006 [2003 May 27].
- [195] Kato T, Kondo T, Bernhardt H, et al. Inventors; Chisso Corp, assignee. Alkenyl compound having a negative deltaepsilon value, liquid crystal composition, and liquid crystal display device. US patent US 7081279 B2. 2006 [2003 Aug 29].
- [196] Kirsch P, Pauluth D, Ruhl A, et al. Inventors; Merck Patent GmbH, assignee. Liquid crystal compounds. US patent US 7135210 B2. 2006 [2004 Apr 15].
- [197] Masukawa T, Fujita A. Inventors; Chisso Corp, Atsuko F. assignee. Tetrahydropyran compounds, liquid crystal compositions, and liquid crystal displays containing the compositions. WO patent WO 2006/038522 A1. 2006 [2005 Sep 29].
- [198] Poetsch E, Lietzau L, Meyer V, et al. Inventors; Merck Patent GmbH, tetrahydropyrane derivatives comprising several rings containing oxygen and method for the production thereof. WO patent WO 2006/125530 A1. 2006 [2006 May 11].
- [199] Reiffenrath V, Heckmeier M, Bremer M. Inventors; Merck Patent GmbH, assignee. Compound having negative deltaepsilon. US patent US 7122228 B2. 2006 [2004 Jan 20].
- [200] Tuffin Rachel P, Goodby John W, Hird M, et al. Inventors; Qinetiq Ltd, assignee. Benzo-1, 3-dioxanes for use in liquid crystal devices. WO patent WO 2006/048620 A3. 2006 [2005 Nov 1].
- [201] Kazutoshi M, Hiroyuki T, Hitoshi Y. Inventors; Chisso Corp, assignee. Liquid crystal compound having negative dielectric anisotropy, liquid crystal composition containing the compound and liquid crystal display element produced by using the composition. JP patent JP 4003244 B2. 2007 [1997 Feb 24].
- [202] Hitoshi Y, Shinichi S, Hiroyuki T, et al. Inventors; Chisso Corp, assignee. Liquid crystalline compound having negative anisotropy value of dielectric constant, liquid crystal composition containing the same and liquid crystal display element using the composition. JP 3991398 B2. 2007 [1997 Oct 8].
- [203] Ban B-S. Inventor; Samsung Electronics Co Ltd, assignee. Nematic liquid crystal composition. US patent US 7220368 B2. 2007 [2006 May 12].
- [204] Bernatz G, Best P, Goetz A, et al. Inventors; Merck Patent GmbH. Mesogenic compounds, liquid crystal medium and liquid crystal display. WO patent WO 2007/147516 A1. 2007 [2007 Jun 14].
- [205] Kirsch P, Hahn A, Poetsch E, et al. Inventors; Merck Patent GmbH, assignee. Liquid-crystalline compounds. US patent US 7291367 B2. 2007 [2005 May 27].
- [206] Melanie Lietzau Lars Bremer MA. Inventor; Merck Patent GmbH, assignee. New as-indacene derivatives. CN patent CN 1947054 A. 2007 [2005 Apr 12].
- [207] Melanie Lietzau Lars Bremer MA. Inventor; Merck Patent GmbH, assignee. Dibenzofuran-, dibenzothiophene- and fluorene derivatives. CN patent CN 1942461 A. 2007 [2005 Mar 18].

- [208] Sasada Y. Inventor; Chisso Corp, assignee. Compound having alkyl group in benzene ring, liquid crystal composition containing the compound and liquid crystal display element containing the liquid crystal composition. JP patent JP 2007099734 A. 2007 [2005 Oct 7].
- [209] Satou T, Kondou T, Hattori N, et al. Inventors; Chisso Corp, assignee. Monofluorinated terphenyl compound having alkenyl, liquid crystal composition and liquid crystal display element. WO patent WO 2007/077844 A1. 2007 [2006 Dec 26].
- [210] Taugerbeck A, Heckmeier M, Kirsch P, et al. Inventors; Merck Patent GmbH, assignee. Cyclobutane derivatives. US patent US 7270856 B2. 2007 [2005 Jun 1].
- [211] Yamashita J, Matsui S. Inventors; Chisso Corp, assignee. Compound having alkadienyl group as side chain, and liquid crystal composition using the same. JP patent JP 2007126449 A. 2007 [2006 Oct 2].
- [212] Byeong Seop B, Bong Hui K, Bong Seong S, et al. Inventors; Samsung Electronics Co Ltd, assignee. Liquid crystal composition comprising isothiocyanate-based compound and liquid crystal display using the same. KR patent KR 100853223 B1. 2008 [2002 Nov 28].
- [213] Yasuyuki K, Hitoshi Y. Inventors; Chisso Corp, assignee. Liquid crystal compound having negative dielectric anisotropy, liquid crystal composition containing the liquid crystal compound and liquid crystal display element produced by using the liquid crystal composition. JP patent JP 4106716 B2. 2008 [1997 Frb 25].
- [214] Shinichi S, Koichi S, Hiroyuki T, et al. Inventors; Chisso Corp, assignee. New liquid crystal compound having difluoromethyleneoxy group, liquid crystal composition, and liquid crystal display element. JP patent JP 4075105 B2. 2008 [1997 Jul 11].
- [215] Jazutoshi M, Hitoshi Y. Inventors; Chisso Corp, assignee. Liquid crystal compound having negative anisotropic value of dielectric constant, liquid crystal composition containing the same and liquid crystal display element using the composition. JP patent JP 4075092 B2. 2008 [1997 Feb 27].
- [216] Hitoshi Y, Demus D. Inventors; Chisso Corp, assignee. Liquid crystal compound having negative anisotropic value of dielectric constant, liquid crystal composition containing the same and liquid crystal display element using the composition. JP patent JP 4048570 B2. 2008 [1997 Feb 25].
- [217] Eike P, Lars L, Volker M, et al. Inventors; Merck Patent GmbH, assignee. Tetrahydropyran derivatives comprising several rings containing oxygen and method for the production thereof. CN patent CN 101180295 A. 2008 [2006 May 11].
- [218] Kirsch P, Poetsch E, Hahn A, et al. Inventors; Merck Patent Gesellschaft Mit, assignee. Liquid-crystalline compounds. US patent US 7344761 B2. 2008 [2004 May 24].
- [219] Kirsch P, Poetsch E, Manabe A. Inventors; Merck Patent GmbH, assignee. Liquid-crystalline compounds having a tetrahydropyran ring. US patent US 7361388 B2. 2008 [2005 Nov 25].
- [220] Kirsch P, Taugerbeck A, Hahn A. Inventors; Merck Patent GmbH, assignee. Process for the preparation of compounds having a CF₂O bridge. US patent US 7385067 B2. 2008 [2006 Jun 2].
- [221] Klein M, Kirsch P, Poetsch E, et al. Inventors; chromane derivatives method for production and the use thereof. US patent US 2008/0020148 A1. 2008. [2005 Sep 28].
- [222] Lars L, Markus C. Inventors; Merck Patent GmbH, assignee. Pyran/dioxan derivatives and use thereof in liquid crystal media. CN patent CN 101180294 A. 2008 [2006 May 3].
- [223] Lars L, Werner B, Eike P, et al. Inventors; Merck Patent GmbH, assignee. Spiro [3.3] heptyl-dioxan derivatives and their use in liquid crystal media. CN patent CN 101291921 A. 2008 [2006 Oct 11].
- [224] Okumura K, Fujita A. Inventors; Chisso Corp, assignee. New compound having 2,2,2-bicyclooctane bonded with halogenated alkyl and liquid crystal composition using the same. JP patent JP 2008247890 A. 2008 [2008 Feb 28].
- [225] Shimada T. Inventor; Chisso Corp, assignee. Cyclohexene derivative having alkenyl group, liquid crystal composition and liquid crystal display device. JP patent JP 2008088165 A. 2008 [2007 Sep 5].
- [226] Xinqin LIU, Jianli Z, Xiao L. Inventors; Shijiazhuang Yongsheng Huatsin, assignee. 2-site ethynyl contained pyrimidine ring liquid crystal compounds and method for preparing the same. CN patent CN 101323596 A. 2008 [2008 Aug 7].
- [227] Yamashita J. Inventor; Chisso Corp, assignee. Alkadienyl-group-containing compound and liquid crystal composition using the same. JP patent JP 2008273957 A. 2008 [2008 Apr 3].
- [228] 益川 解, 藤田 敦. inventors; チッソ石油化学株式会社, チッソ株式会社, assignee. テトラヒドロピラン化合物、液晶組成物およびこの液晶組成物を含む液晶表示素子. JP patent JP WO2006038522 A1. 2008 [2005 Sep 29].
- [229] Harald H, Kevin A, Patricia S, et al. Inventors; Merck Patent GmbH, assignee. Toluene derivatives and liquid crystalline medium. CN patent CN 100569716 C. 2009 [2004 May 21].
- [230] Heckmeier M, Kirsch P, Krause J, et al. Inventors; Merck Patent GmbH, assignee. Liquid-crystalline compounds. US patent US 7604851 B2. 2009. [2007 Jul 23].
- [231] Jansen A, Klasen-Memmer M. Inventors; Merck Patent GmbH, assignee. Benzo[f]chrome and pyrano[3,2-f]chrome derivatives for use in liquid crystal media. WO patent WO 2009/068152 A1. 2009 [2008 Nov 3].
- [232] Kirsch P, Montenegro E, Farrand Louise D, et al. Inventors; Merck Patent GmbH, assignee. Mesogenic compounds, medium for electro-optical displays and electro-optical display. US patent US 7531106 B2. 2009 [2006 Feb 24].
- [233] Kobayashi M, Inventor; Chisso Corp, assignee. Tricyclic liquid crystalline compound having lateral fluorine, liquid crystal composition and liquid crystal display device. WO patent WO 2009/125668. 2009 [2009 Mar 25]; p. A1.
- [234] Kubo T, Shimada T. Inventors; Chisso Corp, assignee. Liquid crystalline tetracyclic compound having fluorine atom, liquid crystal composition and liquid crystal display element. WO patent WO 2009/145101 a1. 2009 [2009 May 21].

- [235] Lars L, Markus C, Atsutaka M, et al. Inventors; Merck Patent GmbH, assignee. New cyclohexene-compounds useful as a component in a liquid crystal medium. CN patent CN 101506330 A. **2009** [2007 Jul 18].
- [236] Lietzau L, Bremer M, Klasen-Memmer M. Inventors; Merck Patent GmbH, assignee. Dibenzofuran derivatives, dibenzothiophene derivatives and fluorene derivatives. US patent US 7514127 B2. **2009** [2005 Mar 18].
- [237] Masukawa T, Inventor; Chisso Corp, assignee. Liquid crystalline compound having negative dielectric anisotropy, liquid crystal composition, and liquid crystal display element. WO patent WO 2009/157313. **2009** [2009 Jun 11]; p. A1.
- [238] Shimada T. Inventor; Chisso Corp, assignee. Liquid crystalline compound, liquid crystal composition, liquid crystal display element. EP patent EP 2123623 A1. **2009** [2008 Jan 15].
- [239] Shimada T, Kobayashi M. Inventors; Chisso Corp, assignee. Liquid crystalline compound, liquid crystal composition, and liquid crystal display element. WO patent WO 2009/034867 A1. **2009** [2008 Sep 1].
- [240] Tanaka H. Inventor; Chisso Corp, assignee. Pentacyclic liquid crystal compound, liquid crystal composition, and liquid crystal display element. JP patent JP 2009292730 a. **2009** [2007 Apr 17].
- [241] Tanaka H. Inventor; Chisso Corp, assignee. Pentacyclic liquid crystal compound having CF₂O bonding group, liquid crystal composition and liquid crystal display. EP patent EP 2116522 A1. **2009** [2008 Feb 20].
- [242] 佐藤 禎, 近藤 智, 服部 憲, et al., inventors; チッソ株式会社, チッソ石油化学株式会社, assignee. アルケニルを有するモノフッ素化テルフェニル化合物、液晶組成物および液晶表示素子. JP patent JP WO2007077844 A1. **2009** [2006 Dec 26].
- [243] Ennis Joanne E, Goodby John W, Tuffin Rachel P, et al. Inventors; QinetiQ Ltd, assignee. Liquid crystal compounds. WO patent WO 2010/012994 A1. **2010** [2009 Jul 29].
- [244] Klasen-Memmer M, Bremer M, Manabe A. Inventors; Merck Patent GmbH, assignee. Stilbene derivatives, liquid-crystal mixtures and electro-optical displays. US patent US 7732022 B2. **2010** [2007 Dec 10].
- [245] Kobayashi M. Inventor; Chisso Corp, assignee. Liquid crystalline compound, liquid crystal composition, and liquid crystal display element. WO patent WO 2010/082558 A1. **2010** [2010 Jan 12].
- [246] Kondou T, Shuichi M, Kimura K. Inventors; Chisso Corp, assignee. Naphthalene compound with terminal hydrogen, liquid crystal composition including the compound, and LCD device including the liquid crystal composition. EP patent EP 1762605 B1. **2010** [2006 Sep 6].
- [247] Lars L, Markus C. Inventors; Merck Patent GmbH, assignee. Pyridine compounds for liquid-crystalline mixtures. CN patent CN 101663275 A. **2010** [2008 Apr 1].
- [248] Lietzau L, Farrand Louise D, Czanta M, et al. Inventors; Merck Patent GmbH, assignee. Thiophene compounds for liquid-crystalline media. WO patent WO 2010/094455 A1. **2010** [2010 Feb 16].
- [249] Reiffenrath V, Bremer M, Klasen-Memmer M. Inventors; Merck Patent GmbH, assignee. Cyclobutane and spiro[3.3]heptane compounds. US patent US 7744968 B2. **2010** [2006 Aug 16].
- [250] Shimada T. Inventor; Chisso Corp, assignee. Liquid crystal compound, liquid crystal composition and, liquid crystal display device. US patent US 7846514 B2. **2010** [2008 Jan 15].
- [251] Shimada T, Yamashita J. Inventors; Chisso Corp, assignee. Liquid crystalline compound having negative dielectric anisotropy, and liquid crystal composition and liquid crystal display element each comprising same. WO patent WO 2010/095493 A1. **2010** [2010 Jan 27].
- [252] 綿田 輝, 小林 雅. inventors; チッソ株式会社, チッソ石油化学株式会社, assignee. 液晶性化合物、液晶組成物および液晶表示素子. JP patent JP WO2009034867 A1. **2010** [2008 Sep 1].
- [253] Ljee Hwan J, Ji Young J, Jong Seob K, et al. Inventors. Samsung Electronic Co Ltd, assignee. Liquid crystalline compound having negative dielectric anisotropy and liquid crystalline composition comprising the same. KR patent KR 101045443 B1. **2011** [2003 Sep 23].
- [254] Hyung Soo C, Byung Soon C, Jong Seob K, et al. Inventors. Samsung Electronics Co Ltd, assignee. Liquid crystal compound with dibenzocycloheptene ring and liquid crystalline composition comprising the same. KR patent KR 101045408 B1. **2011** [2003 Oct 6].
- [255] Goto M, Sugiura T, Hattori N. Inventors; Chisso Corp, assignee. Liquid crystal compound having lactone ring, liquid crystal composition, and liquid crystal display device. US patent US 7875327 B2. **2011** [2009 Oct 2].
- [256] Goto S, Sagou K, Fujita H. Inventors; Chisso Corp, assignee. Liquid crystal compound, liquid crystal composition and liquid crystal display device. US patent US 2011/0180756 A1. **2011** [2011 Jan 24].
- [257] Jasper C, Montenegro E, Pauluth D, et al. Inventors; Merck Patent GmbH, assignee. Compounds for a liquid crystal medium and use thereof for high-frequency components. WO patent WO 2011/054425 A1. **2011** [2010 Oct 6].
- [258] Jasper C, Montenegro E, Pauluth D, et al. Inventors; Merck Patent GmbH, assignee. Compounds for a liquid crystal medium and use for high-frequency components. WO patent WO 2011/047781 A1. **2011** [2010 Oct 1].
- [259] Kobayashi M. Inventor; Kobayashi Masahide, assignee. Four-ring liquid crystal compound having lateral fluorine, liquid crystal composition and liquid crystal display device. US patent US 2011/0090450 A1. **2011** [2009 Jun 2].
- [260] Kobayashi M, Yamashita J. Inventors; Chisso Corp, assignee. Liquid crystalline compound, liquid crystal composition, and liquid crystal display element. WO patent WO 2011/033937 A1. **2011** [2010 Sep 2].
- [261] Kubo T. Inventor; JNC Corp, Chisso Petrochemical Corp, assignee. Indole ring-bearing compound, liquid crystal composition, and liquid crystal display element. JP patent JP 2011184388 A. **2011** [2010 Mar 10].
- [262] Lars L, Werner B, Atsutaka M, et al. Inventors; Merck Patent GmbH, assignee. Liquid crystal compounds. CN patent CN 102050708 A. **2011** [2010 Nov 4].
- [263] Masukawa T. Inventor; Chisso Corp assignee. Liquid crystal compound having negative dielectric anisotropy, liquid crystal composition, and liquid crystal display device. US patent US 7914862 B2. **2011** [2009 May 4].
- [264] Masukawa T. Inventor; Chisso Corp, assignee. Decahydronaphthalene compounds, liquid crystal

- compositions containing the compounds, and liquid crystal display elements containing the liquid crystal compositions. WO patent WO 2011/021525 A1. [2011](#) [2010 Aug 9].
- [265] Matsui S, Sasada Y. Inventors; JNC Corp, Chisso Petrochemical Corp, assignee. Benzene derivative, liquid crystal composition, and liquid crystal display element. JP patent JP 2011173894 A. [2011](#) [2011 Mar 30].
- [266] Okumura K, Kimura K. Inventors; JNC Corp, assignee. Liquid crystal compound comprising condensed ring having two oxygens, and liquid crystal composition using the same. JP patent JP 2011251931 A. [2011](#) [2010 Jun 1].
- [267] Sasada Y. Inventor; JNC Corp, Chisso Petrochemical Corp, assignee. Compound having alkyl on benzene ring, liquid crystal composition having the compound, and liquid crystal display device having the liquid crystal composition. US patent US 7981486 B2. [2011](#) [2009 Mar 18].
- [268] Tanaka H. Inventor; JNC CORP, CHISSO PETROCHEMICAL CORP, Tanaka Hiroyuki, assignee. Liquid crystal compound, liquid crystal composition and liquid crystal display element. WO patent WO 2011/083677 A1. [2011](#) [2010 Dec 20].
- [269] Tanaka H. Inventor; Chisso Corp, assignee. Five-ring liquid crystal compound having cyclohexane ring, liquid crystal composition, and liquid crystal display device. US patent US 7951432 B2. [2011](#) [2009 Jun 4].
- [270] Yamashita J, Kobayashi M, Fujimori S. Inventors; Chisso Corp, assignee. Liquid crystalline compound with negative dielectric anisotropy, liquid crystal composition using same, and liquid crystal display element. WO patent WO 2011/040373 A1. [2011](#) [2010 Sep 27].
- [271] Yano T. Inventor; JNC CORP, assignee. Trans-monofluoroethylene liquid crystal compound having negative dielectric anisotropy, a liquid crystal composition using the compound and a liquid crystal display device. US patent US 2011/0291047 A1. [2011](#) [2011 May 24].
- [272] 久保 貴, 綿田 輝. inventors; JNC CORP, assignee. チッソ石油化学株式会社, assignee. フッ素原子を有する液晶性四環化合物、液晶組成物、及び液晶表示素子. JP patent JP WO2009145101 A1. [2011](#) [2009 May 21].
- [273] 小林 雅. inventor; JNC CORP, assignee. チッソ石油化学株式会社, assignee. ラテラルフッ素を有する3環液晶性化合物、液晶組成物および液晶表示素子. JP patent JP WO2009125668 A1. [2011](#) [2009 Mar 25].
- [274] 益川 解. Inventor; JNC CORP, assignee. 誘電率異方性が負の液晶性化合物、液晶組成物および液晶表示素子. JP patent JP WO2009157313 A1. [2011](#) [2009 Jun 11].
- [275] Shunsuke T, Jiroaki O, Yuki M, et al. Inventors; Chisso Corp, assignee. Benzodioxine derivative, liquid crystal composition containing the same and liquid crystal display element. JP patent JP 4978017 B2. [2012](#) [2006 Feb 9].
- [276] Shotaro K, Takashi M, Tetsuo K, et al. Inventors; Dainippon Ink and Chemicals, assignee. Difluorobenzene derivative and nematic liquid crystal composition using the same. KR patent KR 101158485 B1. [2012](#) [2006 Feb 27].
- [277] Haseba Y, Kuninobu T. Inventors; JNC Corp, assignee. Chlorobenzene derivative, optically isotropic liquid crystal medium, and optical device. US patent US 2012/0099039 A1. [2012](#) [2010 May 7].
- [278] Hirata K, Ookawa H. Inventors; JNC Corp assignee. Compound containing dihydrophenanthrene, liquid crystal composition and liquid crystal display. WO patent WO 2012/086437 A1. [2012](#) [2011 Dec 9].
- [279] Jansen A, Pauluth D, Klasen-Memmer M. Inventors; Merck Patent GmbH, assignee. 2, 5-selenophene derivatives and 2, 5-tellurophene derivatives. US patent US 8304036 B2. [2012](#) [2008 Aug 7].
- [280] Jasper C, Manabe A, Pauluth D, et al. Inventors; Merck Patent GmbH assignee. Compounds for a liquid crystal medium, and the use thereof for high-frequency components. WO patent WO 2012/069133 A1. [2012](#) [2011 Oct 31].
- [281] Jasper C, Montenegro E, Pauluth D, et al. Inventors; Merck Patent GmbH, assignee. Compounds for a liquid crystalline medium and use thereof for high frequency components. WO patent WO 2012/095139 A1. [2012](#) [2011 Dec 14].
- [282] Jianli Z, Xiao L, Xinqin LIU. Inventors; Shijiazhuang Yongsheng Huatsing Liquid Crystal Co Ltd, assignee. 2-site ethynyl contained pyrimidine ring liquid crystal compounds and method for preparing the same. CN patent CN 101323596 B. [2012](#) [2008 Aug 7].
- [283] Kobayashi M. Inventor; JNC CORP, assignee. Five-ring liquid crystal compound, liquid crystal composition and liquid crystal display device. US patent US 2012/0074355 A1. [2012](#) [2010 Jun 2].
- [284] Kubo T, Tanaka H. Inventors; JNC Corp, Chisso Petrochemical Corp, assignee. Compound having propylether moiety in linking group, liquid crystal composition and LCD device. TW patent TW 201211216 A. [2012](#) [2011 Aug 9].
- [285] Reiffenrath V, Jasper C, Manabe A, et al. Inventors; Merck Patent GmbH, assignee. Compounds for a liquid crystal medium and use of said compounds for high-frequency components. WO patent WO 2012/048774 A1. [2012](#) [2011 Sep 14].
- [286] Reiffenrath V, Jasper C, Pauluth D, et al. Inventors; Merck Patent GmbH, assignee. Compounds of liquid crystalline medium and use thereof for high-frequency components. WO patent WO 2012/146340 a1. [2012](#) [2012 Mar 28].
- [287] Sasada Y. Inventor; JNC Corp, assignee. Cyclohexene-3,6-diyl compound, liquid crystal composition, and liquid crystal display element. WO patent WO 2012/053421 A1. [2012](#) [2011 Oct 13].
- [288] Tanaka H. Inventor; Chisso Petrochemical Corp, JNC Corp, assignee. Liquid crystal compound having difluoropropenylenoxy bonding group. US patent US 2012/0029194 A1. [2012](#) [2010 Mar 15].
- [289] 小林 雅. Inventor; JNC CORP, assignee. 液晶性化合物、液晶組成物および液晶表示素子. JP patent JP WO2010082558 A1. [2012](#) [2010 Jan 12].
- [290] Haseba Y. Inventor; JNC CORP, assignee. Chlorofluorobenzene compound, optically isotropic liquid crystal medium and optical device. US patent US 8586803 B2. [2013](#) [2012 Nov 30].
- [291] Hou Z, Yuan G, Zhang X, et al. Inventors; Shijiazhuang Chengzhi Yonghua Display Materials Co Ltd, assignee. Liquid crystal compound containing cyclobutyl and

- difluorometheneoxy. CN patent CN 103242855 A. **2013** [2013 May 15].
- [292] Kobayashi M. Inventor; JNC Corp, assignee. Compound having bicyclo[3.3.0]octane-2,6-diyl, liquid crystal composition and liquid crystal display device. US patent US 8585924 B2. **2013** [2012 May 10].
- [293] Kobayashi M. Inventor; JNC Corp, assignee. Liquid crystal compound, liquid crystal composition and liquid crystal display device. US patent US 8580146 B2. **2013** [2012 Jan 27].
- [294] Kobayashi M, Shimada T. Inventors; JNC Corp assignee. Tetra- or penta-cyclic liquid crystalline compound having lateral fluorine, liquid crystal composition, and liquid crystal display element. EP patent EP 2206695 B1. **2013** [2008 Aug 26].
- [295] Kubo T, Goto Y. Inventors; JNC Corp, assignee. Four-ring compound having a plurality of CF₂O bonding groups, liquid crystal composition and liquid crystal display device. US patent US 8603359 B2. **2013** [2012 Jun 6].
- [296] Lietzau L, Czanta M, Manabe A. Inventors; Merck Patent GmbH, assignee. Tetrahydropyran compounds. US patent US 8465672 B2. **2013** [2007 Jul 17].
- [297] Lv W, Yuan G, Wang J, et al. Inventors; Shijiazhuang Chengzhi Yonghua Display Materials Co Ltd, assignee. Liquid crystal compound containing difluoro-methylene key bridge, preparation method thereof and composition containing liquid crystal compound. CN patent CN 103254903 A. **2013** [2013 Apr 27].
- [298] Maeda T, Yanai T, Tanaka H, et al. Inventors; JNC Corp, assignee. Compound, liquid crystal composition and liquid crystal display device. US patent US 8592008 B2. **2013** [2012 Jun 11].
- [299] Sasaki T, Takebe Y, Ito M. Inventors; Asahi Glass Co Ltd, assignee. Fluorine-containing aromatic compound, organic semiconductor material and organic thin film device. US patent US 2013/0119363 a1. **2013** [2013 Jan 4].
- [300] Tanaka H. Inventor; JNC Corp, assignee. Liquid crystal compound having tetrafluoropropenyl, liquid crystal composition, and liquid crystal display element. WO patent WO 2013/125356 A1. **2013** [2013 Feb 7].
- [301] Xia Z, Hua R, Han Y, et al. Inventors; Shijiazhuang Chengzhi Yonghua Display Materials Co Ltd, assignee. Liquid-crystal compound containing 1,4-dioxo-six-membered ring as well as preparation method and application thereof. CN patent CN 103333155 A. **2013** [2013 Jun 20].
- [302] Yuan G, Xia Z, Liang Z, et al. Inventors; Shijiazhuang Chengzhi Yonghua Display Materials Co Ltd, assignee. Liquid crystal compound containing indan and difluoro methylenedioxy bridge, as well as preparation method and application thereof. CN patent CN 103058836 A. **2013** [2013 Jan 18].
- [303] 小林 雅, 山下 淳. Inventors; JNC CORP, assignee. 液晶性化合物、液晶組成物および液晶表示素子. JP patent JP WO2011033937 A1. **2013** [2010 Sep 2].
- [304] 山下 淳, 小林 雅, 藤森 さ. inventors; JNC CORP, assignee. 誘電率異方性が負の液晶性化合物、これを用いた液晶組成物および液晶表示素子. JP patent JP WO2011040373 A1. **2013** [2010 Sep 27].
- [305] 田中 裕. Inventor; JNC CORP, assignee. 液晶化合物、液晶組成物および液晶表示素子. JP patent JP WO2011083677 A1. **2013** [2010 Dec 20].
- [306] 益川 解. inventor; JNC CORP, assignee. デカヒドロナフタレン化合物、この化合物を含有する液晶組成物およびこの液晶組成物を含有する液晶表示素子. JP patent JP WO2011021525 A1. **2013** [2010 Aug 9].
- [307] Brocke C, Jasper C, Pauluth D, et al. Inventors; Merck Patent GmbH, assignee. Compounds having a C-C triple bond and use thereof in liquid-crystal mixtures. WO patent WO 2014/044357 A1. **2014** [2013 Sep 3].
- [308] Cao J, Wang S, Jia L, et al. Inventors; Shijiazhuang Chengzhi Yonghua Display Materials Co Ltd, assignee. Liquid crystal compound containing tetrahydropyran difluoro methoxy-linking group and preparation method and application thereof. CN patent CN 103788039 A. **2014** [2014 Mar 12].
- [309] Goto M, Sugiura T, Hattori N, et al. Inventors; JNC Corp, assignee. Compound having hydrocoumarin skeleton, liquid crystal composition and liquid crystal display element. EP patent EP 1958945 B1. **2014** [2006 Dec 8].
- [310] Gotoh Y, Kobayashi M. Inventors; JNC Corp, assignee. Liquid crystal compound having vinyloxy, liquid crystal composition and liquid crystal display device. US patent US 2014/0138582 A1. **2014** [2013 Nov 15].
- [311] Haseba Y, Sago K, Yamamoto S-I. Inventors; JNC Corp, assignee. Liquid-crystal compound, liquid-crystalline medium and optical element. WO patent WO 2014/065293 A1. **2014** [2013 Oct 22].
- [312] Jiang T, Hang D, Tian H, et al. Inventors; Beijing Bayi Space LCD Materials Technology Co Ltd, assignee. Liquid crystal compound containing tetrahydropyran ring and application of liquid crystal compound. CN patent CN 104003964 A. **2014** [2014 Jun 6].
- [313] Jiang T, Hang D, Tian H, et al. Inventors; Beijing Bayi Space LCD Materials Technology Co Ltd, assignee. Liquid crystal compound containing terphenyl/quaterphenyl structure and application thereof. CN patent CN 104003852 A. **2014** [2014 Jun 6].
- [314] Jiang T, Hang D, Tian H, et al. Inventors; Beijing Bayi Space LCD Materials Technology Co Ltd, assignee. Liquid crystal compound and its preparation method and use. CN patent CN 104004527 A. **2014** [2014 May 7].
- [315] Jiang T, Tian H, Chu S, et al. Inventors; Beijing Bayi Space LCD Materials Technology Co Ltd, assignee. Liquid crystal chemical compound containing dioxane ring and application thereof. CN patent CN 104099105 A. **2014** [2014 Jun 30].
- [316] Manabe A, Klass D, Seeger R, et al. Inventors; Merck Patent GmbH, assignee. Liquid-crystalline media, components for high-frequency technology, and mesogenic compounds. WO patent WO 2014/094973 A1. **2014** [2013 Dec 2].
- [317] Masukawa T. Inventor; JNC Corp, assignee. Ortho ester derivative, liquid crystal composition, and liquid crystal display device. EP patent EP 2690103 A1. **2014** [2012 Mar 7].
- [318] Satou T, Goto Y. Inventors; JNC Corp, assignee. Fluorovinyl derivative, liquid crystal composition and liquid crystal display device. US patent US 8765011 B2. **2014** [2012 May 10].
- [319] Zhang J, Shao ZHE, Han Y, et al. Inventors; Shijiazhuang Chengzhi Yonghua Display Materials Co Ltd, assignee. Liquid crystal compound containing tetrahydro-thiopyran group and preparation method

- thereof, and liquid crystal composition. CN patent CN 103555344 A. **2014** [2013 Oct 10].
- [320] 平田 健, 大川 裕. inventors; JNC CORP, assignee. ジヒドロフェナントレンを有する化合物、液晶組成物および液晶表示素子. JP patent JP WO2012086437 A1. **2014** [2011 Dec 9].
- [321] 笹田 康. inventor; JNC CORP, assignee. シクロヘキセン-3, 6-ジイル化合物、液晶組成物および液晶表示素子. JP patent JP WO2012053421 A1. **2014** [2011 Oct 13].
- [322] Kenta T, Tetsuo K, Masashi O, et al. Inventors; Dainippon Ink and Chemicals, assignee. Compound having 2-fluorophenyloxymethane structure. KR patent KR 101488315 B1. **2015** [2013 Apr 24].
- [323] Deng JIA, Yun G, Li M, et al. Inventors; Shijiazhuang Chengzhi Yonghua Display Materials Co Ltd, assignee. Liquid crystal compound and liquid crystal mixture containing same. CN patent CN 104402683 A. **2015** [2014 Nov 21].
- [324] Deng JIA, Yun G, Li M, et al. Inventors; Shijiazhuang Chengzhi Yonghua Display Materials Co Ltd, assignee. Liquid crystal compound, and preparation method and application thereof. CN patent CN 105176542 A. **2015** [2015 Sep 2].
- [325] Fujimori S. Inventor; JNC CORP, assignee. 1,3-dioxane compound having fluorine atom in axial position, liquid crystal composition and liquid crystal display device. US patent US 2015/0368225 A1. **2015** [2015 Jun 18].
- [326] Goto M. Inventor; JNC Corp, assignee. Carbonyl derivative, liquid crystal composition containing compound thereof and liquid crystal display device. US patent US 2015/0218452 A1. **2015** [2015 Feb 5].
- [327] Goto M, Fujimori S. Inventors; JNC Corp, assignee. Liquid crystal compound showing negative dielectric anisotropy, liquid crystal composition and liquid crystal display device. US patent US 9102871 B2. **2015** [2013 Apr 18].
- [328] Goto M, Hirata K, Sasada Y. Inventors; JNC Corp, assignee. Dihydropyran compound, liquid crystal composition and liquid crystal display device. US patent US 2015/0252264 A1. **2015** [2015 Mar 4].
- [329] Gotoh Y, Kimura K. Inventors; JNC Corp, assignee. Liquid crystal compound having fluorovinyl group, liquid crystal composition and liquid crystal display device. US patent US 8956551 B2. **2015** [2013 Jul 10].
- [330] Gotoh Y, Kobayashi M. Inventors; JNC Corp, assignee. Liquid crystal compound, liquid crystal composition and liquid crystal display device. US patent US 2015/0368272 A1. **2015** [2015 Jun 24].
- [331] Gotoh Y, Yano M. Inventors; JNC Corp, assignee. Compound having 3,3-difluoro-1-propenyloxy, liquid crystal composition and liquid crystal display device. US patent US 2015/0060732 A1. **2015** [2014 Aug 27].
- [332] Han W, Song X, Yan J, et al. Inventors; Jiangsu Hecheng Display Tech, assignee. Difluorometheneoxy-containing liquid crystal compound, composition and applications thereof. CN patent CN 104788297 A. **2015** [2014 Jan 16].
- [333] Kobayashi M. Inventor; JNC CORP, assignee. Liquid crystal compound having fluorine-containing alkenyl terminal group, liquid crystal composition and liquid crystal display device. US patent US 2015/0232759 A1. **2015** [2015 Feb 18].
- [334] Kobayashi T, Kubo T, Sasada Y. Inventors; JNC Corp, assignee. Dihydropyran compound, liquid crystal composition and liquid crystal display device. US patent US 2015/0361344 a1. **2015** [2015 Jun 11].
- [335] Kubo T, Gotoh Y. Inventors; JNC Corp, assignee. Tricyclic compound having a plurality of CF₂O bonding groups, liquid crystal composition, and liquid crystal display device. US patent US 9133397 B2. **2015** [2013 Apr 4].
- [336] Li M, Shang H, Meng J, et al. Inventors; Shijiazhuang Chengzhi Yonghua Display Materials Co Ltd, assignee. Liquid crystal compound containing methylbenzene and difluoro methyleneoxy linking group and preparing method and application thereof. CN patent CN 105130767 A. **2015** [2015 Sep 2].
- [337] Reiffenrath V, Bremer M, Fortte R, et al. Inventors; Merck Patent GmbH, assignee. 4,6-difluorodibenzofuran derivatives. US patent US 2015/0259602 A1. **2015** [2015 Mar 17].
- [338] Sagou K, Haseba Y. Inventors; JNC Corp, assignee. Compound having branched alkyl or branched alkenyl, optically isotropic liquid crystal medium and optical element. EP patent EP 2586764 A4. **2015** [2011 Jun 15].
- [339] Takahashi M, Fujimori S, Sasada Y. Inventors; JNC Corp, assignee. Liquid crystal compound having CF₂O bonding group and tolane backbone, liquid crystal composition, and liquid crystal display element. WO patent WO 2015/190399 A1. **2015** [2015 Jun 4].
- [340] Takata A, Kubo T. Inventors; JNC Corp, assignee. Liquid crystal compound having 1,1,3,3-tetrafluoroalkyloxy group, liquid crystal composition, and liquid crystal display element. WO patent WO 2015/129540 a1. **2015** [2015 Feb 19].
- [341] Tanaka H, Endou H. Inventors; JNC Corp, assignee. Liquid crystal compound, liquid crystal composition, and liquid crystal display element. EP patent EP 2960226 A1. **2015** [2014 Jan 27].
- [342] Tanaka H, Fujimori S. Inventors; JNC Corp, assignee. Liquid crystal compound having perfluoroalkyl chain, and liquid crystal composition and liquid crystal display device. US patent US 8999196 B2. **2015** [2012 Aug 23].
- [343] Wang C-C, Hsieh Y-Y, Yu H-J. Inventors; Daxin Materials Corp, assignee. Liquid crystal compound having negative dielectric anisotropy, and liquid crystal composition. US patent US 9133396 B2. **2015** [2013 Oct 8].
- [344] Wang JIN, Hua R, Yuan G, et al. Inventors; Shijiazhuang Chengzhi Yonghua Display Materials Co Ltd, assignee. Liquid crystal compound and liquid crystal mixture containing same. CN patent CN 104529907 A. **2015** [2014 Dec 31].
- [345] Yuan G, Zhang X, Wang JIN, et al. Inventors; Shijiazhuang Chengzhi Yonghua Display Materials Co Ltd, assignee. Liquid crystal compound and liquid crystal mixture containing same. CN patent CN 104610976 A. **2015** [2014 Dec 31].
- [346] 도조 겐, 구스모토 데. Inventors; 디아이씨 가부시끼 가이샤, assignee. Compound having fluorinated naphthalene structure and liquid crystal composition

- of said compound. KR patent KR 101576962 B1. [2015](#) [2013 Sep 19].
- [347] 榎原 雅, 高木 一, 美坐 譲. Inventors; 積水樹脂株式会社, assignee. 内照式標示体. JP patent JP 5828781 B2. [2015](#) [2012 Mar 1].
- [348] 田中 裕. inventor; JNC CORP, assignee. テトラフルオロプロベニルを有する液晶性化合物、液晶組成物、および液晶表示素子. JP patent JP WO2013125356 A1. [2015](#) [2013 Feb 7].
- [349] Cao J, Hua R. Inventors; Shijiazhuang Chengzhi Yonghua Display Materials Co Ltd, assignee. Liquid crystal compound containing tetrahydropyran difluoro methylene oxygen group and preparation method and application thereof. CN patent CN 105238415 A. [2016](#) [2015 Nov 9].
- [350] Fujimori S. Inventor; JNC Corp, assignee. Liquid crystal compound having xanthene skeleton and exhibiting negative dielectric anisotropy, liquid crystal composition and liquid crystal display device. US patent US 2016/0068754 A1. [2016](#) [2014 Mar 25].
- [351] Goto M, Sasada Y. Inventors; JNC Corp, assignee. Phenolic compound having carbonyl as neighboring group and application thereof. US patent US 9523036 B2. [2016](#) [2013 May 17].
- [352] Goto M, Tanaka H. Inventors; JNC Corp, assignee. Liquid crystal compound, liquid crystal composition and liquid crystal display device. US patent US 9518222 B2. [2016](#) [2015 Aug 6].
- [353] Gotoh Y, Ookawa H. Inventors; JNC Corp, assignee. Compound having 2,2-difluorovinyl group or 1,2,2-trifluorovinyl group, liquid crystal composition and liquid crystal display device. US patent US 9273245 B2. [2016](#) [2013 Jul 1].
- [354] Han Y, Jia G, Huo X. Inventors; Fuyang Sineva Mat Tech Co Ltd, assignee. Compound, liquid crystal composition and liquid crystal display. CN patent CN 106083538 A. [2016](#) [2016 Jun 7].
- [355] Han Y, Liu C, Ding X, et al. Inventors; Fuyang Xinyihua Mat Tech Co Ltd, assignee. Compound, liquid crystal composition, and liquid crystal display. CN patent CN 105669595 A. [2016](#) [2015 Dec 28].
- [356] Li M, Zhang X, Yuan G, et al. Inventors; Shijiazhuang Chengzhi Yonghua Display Materials Co Ltd, assignee. Liquid crystal compound containing 5-cyclobutyl-1,3-dioxy cyclohexane structure, preparation method and applications thereof. CN patent CN 105481824 A. [2016](#) [2014 Sep 16].
- [357] Ookawa H. Inventor; JNC Corp, assignee. Compound having saturated six-membered ring and alkoxy group or alkoxyalkyl group, liquid crystal composition and liquid crystal display element. WO patent WO 2016/133035 A1. [2016](#) [2016 Feb 15].
- [358] Sasada Y. Inventor; JNC Corp, assignee. Liquid crystal compound, liquid crystal composition and liquid crystal display device. US patent US 9309463 B2. [2016](#) [2013 Sep 10].
- [359] Sato S, Hirata K, Kubo T. Inventors; JNC Corp, assignee. Liquid crystal compound having halogenated alkyl, liquid crystal composition, and liquid crystal display element. JP patent JP 2016175886 A. [2016](#) [2015 Mar 23].
- [360] Seo Young HO, Lee Seng KUE, Kim Bong HEE, et al. Inventors; Dongjin Semichem Co Ltd, Beijing Bayi Space LCD Tech Co Ltd, assignee. Liquid crystal compound and liquid crystal composition comprising same. WO patent WO 2016/108442 A3. [2016](#) [2015 Dec 2].
- [361] Tanaka H, Endou H. Inventors; JNC Corp, assignee. Liquid-crystalline compound having difluoromethyleneoxy group, liquid crystal composition, and liquid crystal display element. EP patent EP 2957554 A4. [2016](#) [2014 Jan 27].
- [362] Tanaka H, Hirata K, Yano M. Inventors; JNC Corp, assignee. Liquid crystal compound having tetrafluorofluorene, liquid crystal composition and liquid crystal display device. US patent US 2016/0376503 A1. [2016](#) [2015 Feb 4].
- [363] Tanaka H, Sagou K. Inventors; JNC Corp, assignee. Pentacyclic liquid crystal compound having nitrogen-containing heterocyclic ring, liquid crystal composition, and liquid crystal display device. EP patent EP 2351741 B1. [2016](#) [2009 Oct 14].
- [364] Tanaka H, Sasada Y. Inventors; JNC Corp, assignee. Liquid crystal compound, liquid crystal composition and liquid crystal display device. US patent US 9441161 B2. [2016](#) [2015 Jul 30].
- [365] Tanaka H, Sasada Y. Inventors; JNC Corp, assignee. Liquid crystalline compound, liquid crystal composition and liquid crystal display element. JP patent JP 2016034933 A. [2016](#) [2015 Jul 21].
- [366] Tian H, Jiang T, Chu S, et al. Inventors; Beijing Bayi Space LCD Mat Tech Co Ltd, assignee. Liquid crystal compound, liquid crystal composition and application thereof. CN patent CN 106146250 A. [2016](#) [2015 May 22].
- [367] Yuan G, Liang Z, Wang KUI, et al. Inventors; Shijiazhuang Chengzhi Yonghua Display Materials Co Ltd, assignee. Liquid crystal compound containing cyclopentyl and difluorometheneoxy linking group, preparation method and application thereof. US patent US 9303208 B2. [2016](#) [2013 Jan 18].
- [368] Yun G, Hua R, Wang KUI, et al. Inventors; Shijiazhuang Chengzhi Yonghua Display Materials Co Ltd, assignee. Liquid crystal compound containing cyclobutyl group and difluoromethyleneoxy linking group, and preparation method and use thereof. US patent US 9481828 B2. [2016](#) [2013 Nov 26].
- [369] 矢野 智, 山下 淳. Inventors; JNC CORP, assignee. 末端に c f 2 o c f 3 を有する液晶化合物、液晶組成物および液晶表示素子. JP patent JP 5850023 B2. [2016](#) [2013 Oct 30].
- [370] 長谷場 康, 佐郷 弘, 山本 真. Inventors; JNC CORP, assignee. 液晶化合物、液晶媒体および光素子. JP patent JP WO2014065293 A1. [2016](#) [2013 Oct 22].
- [371] Chu S, Gao L, Jiang T, et al. Inventors; Beijing Bayi Space LCD Mat Tech Co Ltd, assignee. Negative dielectric anisotropic liquid crystal compound and composition and application thereof. CN patent CN 106928033 A. [2017](#) [2015 Dec 30].
- [372] Chu S, Gao L, Jiang T, et al. Inventors; Beijing Bayi Space LCD Mat Tech Co Ltd, assignee. Cyclopentyl and trifluoromethyl structure contained liquid crystal compound and application thereof. CN patent CN 106929036 A. [2017](#) [2015 Dec 30].

- [373] Chu S, Gao L, Tian H, et al. Inventors; Beijing Bayi Space LCD Materials Technology Co Ltd, assignee. Cyclopropyl negative dielectric anisotropy liquid crystal compound and application thereof. CN patent CN 107286951 A. [2017](#) [2016 Apr 1].
- [374] Ding X, Jia G, Ge Q, et al. Inventors; Fuyang Sineva Mat Tech Co Ltd, assignee. Aromatic liquid crystal compound and preparation method, liquid crystal composition and application thereof. CN patent CN 107011919 A. [2017](#) [2017 Mar 6].
- [375] Gao L, Chu S, Tian H, et al. Inventors; Beijing Bayi Space LCD Materials Technology Co Ltd, assignee. Cyclopropyl type negative dielectric anisotropic liquid crystal compound and application thereof. CN patent CN 107400516 A. [2017](#) [2016 May 19].
- [376] Gao L, Chu S, Tian H, et al. Inventors; Beijing Bayi Space LCD Materials Technology Co Ltd, assignee. Cyclopentyl type negative dielectric anisotropic liquid crystal compound, and composition and application thereof. CN patent CN 107400517 A. [2017](#) [2016 May 19].
- [377] Gao L, Chu S, Tian H, et al. Inventors; Beijing Bayi Space LCD Materials Technology Co Ltd, assignee. Cyclopropyl negative dielectric anisotropy liquid crystal compound and application thereof. CN patent CN 107286952 A. [2017](#) [2016 Apr 1].
- [378] Gao L, Chu S, Tian H, et al. Inventors; Beijing Bayi Space LCD Materials Technology Co Ltd, assignee. Cyclopentyl liquid crystal compound, composition, and application of cyclopentyl liquid crystal compound or composition. CN patent CN 107286950 A. [2017](#) [2016 Apr 1].
- [379] Gao L, Chu S, Tian H, et al. Inventors; Beijing Bayi Space LCD Materials Technology Co Ltd, assignee. Cyclopentyl negative dielectric anisotropy liquid crystal compound, composition, and application of cyclopentyl liquid crystal compound or composition. CN patent CN 107286953 A. [2017](#) [2016 Apr 1].
- [380] Goto M. Inventor; JNC Corp, assignee. Carbonyl derivative, liquid crystal composition containing compound thereof and liquid crystal display device. US patent US 9783481 B2. [2017](#) [2015 Feb 5].
- [381] Goto M. Inventor; JNC Corp, assignee. Compound having anthracene skeleton, liquid crystal composition and liquid crystal display element. JP patent JP 2017007986 A. [2017](#) [2015 Jun 24].
- [382] Goto M. Inventor; JNC Corp, assignee. Compound having dihydroanthracene skeleton, liquid crystal composition and liquid crystal display element. JP patent JP 2017007987 A. [2017](#) [2015 Jun 24].
- [383] Gotoh Y, Goto M, Sawada M. Inventors; JNC Corp, assignee. Compound having tetrahydropyran ring, liquid crystal composition and liquid crystal display device. US patent US 2017/0101582 A1. [2017](#) [2016 Oct 5].
- [384] Jiang YI, Xu H, Song X, et al. Inventors; UNIV SHAANXI CHINESE MEDICINE, assignee. Laterally tetrafluoro-substituted dibenzoheterocyclic compound and preparation method thereof. CN patent CN 106699710 A. [2017](#) [2016 Dec 12].
- [385] Kimura K, Kobayashi T. Inventors; JNC Corp, assignee. Liquid crystal compound having tetracycle, liquid crystal composition and liquid crystal display device. US patent US 9777219 B2. [2017](#) [2016 May 16].
- [386] Klasen-Memmer M, Bremer M, Schneider K. Inventors; Merck Patent Ges Mit Beschränkter Haftung, assignee. Liquid crystalline medium. US patent US 9777216 B2. [2017](#) [2011 Jan 31].
- [387] Kubo T, Kobayashi M. Inventors; JNC Corp, assignee. Liquid crystal compound having cyclohexene ring, liquid crystal composition and liquid crystal display device. US patent US 9663717 B2. [2017](#) [2016 Mar 24].
- [388] Li X. Inventor; Fuyang Sineva Mat Tech Co Ltd, assignee. Compound, liquid crystal composition and liquid crystal display. CN patent CN 106543178 A. [2017](#) [2015 Sep 16].
- [389] Li Z. Inventor; Fuyang Sineva Mat Tech Co Ltd, assignee. Compound, liquid crystal composition and liquid crystal display. CN patent CN 106520140 A. [2017](#) [2015 Sep 10].
- [390] Masukawa T, Hirata K, Yamashita J. Inventors; JNC Corp, assignee. Tetrahydropyran compound, liquid crystal composition and liquid crystal display device. US patent US 9663716 B2. [2017](#) [2010 Aug 10].
- [391] Mori A, Kimura K, Satou T. Inventors; JNC Corp, assignee. Tetracyclic liquid crystalline compound having two atom-bonded group and 2, 3-difluorophenylene, liquid crystal composition and liquid crystal display element. WO patent WO 2017/126275 A1. [2017](#) [2016 Dec 19].
- [392] Okumura K, Hirata K. Inventors; JNC CORP, assignee. Alkenyl dioxane compound, liquid crystal composition and liquid crystal display device. US patent US 9657230 B2. [2017](#) [2016 Mar 16].
- [393] Ookawa H, Takata A, Sago K. Inventors; JNC Corp, assignee. Optically isotropic liquid crystal medium and optical device. US patent US 9701904 B2. [2017](#) [2015 Dec 28].
- [394] Sasada Y. Inventor; JNC Corp, assignee. Liquid crystalline compound, liquid crystal composition and liquid crystal display element. JP patent JP 2017137240 A. [2017](#) [2016 Feb 1].
- [395] Sasada Y. Inventor; JNC Corp, assignee. Liquid crystal compound, liquid crystal composition and liquid crystal display device. US patent US 2017/0009137 A1. [2017](#) [2016 Jul 6].
- [396] Satou T, Tachinami S. Inventors; JNC Corp, assignee. Liquid crystal compound having a 3,6-dihydro-2H-pyran ring, negative dielectric anisotropy, liquid crystal composition and liquid crystal display device. US patent US 9790427 B2. [2017](#) [2016 Feb 4].
- [397] Tian H, Chu S, Gao L, et al. Inventors; Beijing Bayi Space LCD Materials Technology Co Ltd, assignee. Isobutyl negative dielectric anisotropic liquid crystal compound and application thereof. CN patent CN 107345140 A. [2017](#) [2016 May 6].
- [398] Tian H, Chu S, Gao L, et al. Inventors; Beijing Bayi Space LCD Materials Technology Co Ltd, assignee. Isopentyl negative dielectric anisotropic liquid crystal compound and application thereof. CN patent CN 107345139 A. [2017](#) [2016 May 6].
- [399] Tian H, Chu S, Gao L, et al. Inventors; Beijing Bayi Space LCD Materials Technology Co Ltd, assignee. Isopentyl negative dielectric anisotropic liquid crystal

- compound and application thereof. CN patent CN 107345141 A. [2017](#) [2016 May 6].
- [400] Tian H, Chu S, Gao L, et al. Inventors; Beijing Bayi Space LCD Materials Technology Co Ltd, assignee. Cyclopentyl negative dielectric anisotropy liquid crystal compound and application thereof. CN patent CN 107286949 A. [2017](#) [2016 Apr 1].
- [401] Tian H, Jiang T, Chu S, et al. Inventors; Beijing Bayi Space LCD Mat Tech Co Ltd, assignee. Liquid crystal compound, composition and applications of liquid crystal compound and composition. CN patent CN 106883861 A. [2017](#) [2015 Dec 16].
- [402] Tian H, Jiang T, Chu S, et al. Inventors; Beijing Bayi Space LCD Mat Tech Co Ltd, assignee. Liquid crystal compound, liquid crystal composition and application of liquid crystal compound and liquid crystal composition. CN patent CN 106811209 A. [2017](#) [2015 Nov 30].
- [403] Tian H, Jiang T, Chu S, et al. Inventors; Beijing Bayi Space LCD Mat Tech Co Ltd, assignee. Liquid crystal compound, liquid crystal composition and application of liquid crystal compound and liquid crystal composition. CN patent CN 106811208 A. [2017](#) [2015 Nov 30].
- [404] Yano M, Tanaka H, Kondo F, et al. Inventors; JNC Corp, assignee. Polar compound, liquid crystal composition and liquid crystal display element. JP patent JP 2017025007 A. [2017](#) [2015 Jul 17].
- [405] Zhang WEI, Meng J, Yun G, et al. Inventors; Shijiazhuang Chengzhi Yonghua Display Materials Co Ltd, assignee. Liquid crystal compound containing dimethylbenzene and difluoromethyleneoxy linking group and application of liquid crystal compound. CN patent CN 107312549 A. [2017](#) [2015 Sep 2].
- [406] 高橋 道, 藤森 さ, 笹田 康. inventors; JNC CORP, assignee. C F 2 O 結合基とトラン骨格を有する液晶化合物、液晶組成物および液晶表示素子. JP patent JP WO2015190399 A1. [2017](#) [2015 Jun 4].
- [407] 高田 章, 久保 貴. inventors; JNC CORP, assignee. 1, 1, 3, 3-テトラフルオロアリルオキシ基を有する液晶性化合物、液晶組成物、および液晶表示素子. JP patent JP WO2015129540 A1. [2017](#) [2015 Feb 19].
- [408] Brocke C, Jasper C, Pauluth D, et al. Inventors; Merck Patent GmbH, assignee. Compounds having a C—C triple bond and use thereof in liquid-crystal mixtures. US patent US 9868905 B2. [2018](#) [2013 Sep 3].
- [409] Gotoh Y, Kubo T. Inventors; JNC CORP, assignee. Compounds having a difluorocyclohexane ring, liquid crystal compositions and liquid crystal display devices. US patent US 10100251 B2. [2018](#) [2017 Feb 22].
- [410] Jang Hye LIM, Shin B-S, Kim SH, et al. Inventors; Samsung Display Co Ltd, assignee. Compound, liquid crystal composition including the same, and liquid crystal display device including the same. US patent US 9862886 B2. [2018](#) [2016 Jun 16].
- [411] Jasper C, Brocke C, Pauluth D, et al. Inventors; Merck Patent GmbH, assignee. Alkynyl-tolanes, liquid-crystal mixtures containing them and components for high-frequency technology. US patent US 10099975 B2. [2018](#) [2014 Aug 11].
- [412] Kobayashi M. Inventor; JNC CORP, assignee. Liquid crystal compound having butene-bonding group, liquid crystal composition and liquid crystal display device. US patent US 10047293 B2. [2018](#) [2015 Aug 7].
- [413] Lietzau L, Brocke C, Reiffenrath V, et al. Inventors; Merck Patent GmbH, assignee. Fluorinated dibenzofuran and dibenzothiophene derivatives. US patent US 10017695 B2. [2018](#) [2016 Apr 11].
- [414] Lo C-Y, Liu H-C, Lan G-Y, et al. Inventors; Daxin Materials Corp, assignee. Liquid crystal compound and liquid crystal composition employing the same. US patent US 10113116 B2. [2018](#) [2016 Jan 27].
- [415] Shi Z, Feng P, Luan Z, et al. Inventors; Yantai Fengpeng LCD Mat Co Ltd, assignee. Liquid crystal composition with negative dielectric anisotropy and preparation method and application thereof. CN patent CN 108517216 A. [2018](#) [2018 Jun 8].
- [416] Takahashi M, Fujimori S, Sasada Y. Inventors; JNC Corp, assignee. Liquid crystal compound, liquid crystal composition and liquid crystal display device. TW patent TW I629343 B. [2018](#) [2015 Jun 10].
- [417] Tanaka H, Takata A. Inventors; JNC Corp, assignee. Liquid crystal compound having tercyclohexyl, liquid crystal composition and liquid crystal display device. US patent US 9994770 B2. [2018](#) [2017 Mar 8].
- [418] Tian H, Jiang T, Chu S, et al. Inventors; Beijing Bayi Space LCD Materials Technology Co Ltd, assignee. Negative-dielectric anisotropic liquid crystal compound, preparation method thereof and application of compound. CN patent CN 109082281 A. [2018](#) [2017 Jun 14].
- [419] Tian H, Jiang T, Tan X, et al. Inventors; Beijing Bayi Space LCD Materials Technology Co Ltd, assignee. Liquid crystal compound with negative dielectric anisotropy as well as preparation method and application thereof. CN patent CN 108728112 A. [2018](#) [2017 Apr 19].
- [420] Tian H, Tan X, Chu S, et al. Inventors; Beijing Bayi Space LCD Materials Technology Co Ltd, assignee. 2,3-difluorobenzene negative dielectric anisotropy liquid crystalline compound as well as preparation method and application thereof. CN patent CN 108530275 A. [2018](#) [2017 Mar 2].
- [421] Yano T. Inventor; JNC Corp, assignee. Liquid crystal compound having benzothiophene, liquid crystal composition and liquid crystal display device. US patent US 2018/0290997 A1. [2018](#) [2016 Jul 11].
- [422] 森 紘, 木村 敬, 佐藤 禎. inventors; JNC CORP, assignee. 2 原子結合基と 2, 3-ジフルオロフェニレンを有する 4 環液晶性化合物、液晶組成物および液晶表示素子. JP patent JP WO2017126275 A1. [2018](#) [2016 Dec 19].
- [423] Gao L, Jiang T, Chu S, et al. Inventors; Beijing Bayi Space LCD Materials Technology Co Ltd, assignee. Dibenzothiophene liquid crystal compound, and preparation method and application thereof. CN patent CN 109423297 A. [2019](#) [2017 Aug 24].
- [424] Gao L, Jiang T, Chu S, et al. Inventors; Beijing Bayi Space LCD Materials Technology Co Ltd, assignee. Novel dibenzothiophene liquid crystal compound, and preparation method and application thereof. CN patent CN 109423298 A. [2019](#) [2017 Aug 25].

- [425] Gao L, Jiang T, Chu S, et al. Inventors; Beijing Bayi Space LCD Materials Technology Co Ltd, assignee. Liquid crystal compound containing alkenes and with negative dielectric anisotropy and application thereof. CN patent CN 109207158 A. [2019](#) [2017 Jun 29].
- [426] Gao L, Jiang T, Chu S, et al. Inventors; Beijing Bayi Space LCD Materials Technology Co Ltd, assignee. Negative dielectric anisotropic liquid crystal compound, preparation method and application thereof. CN patent CN 109207159 A. [2019](#) [2017 Jun 30].
- [427] Haseba Y, Sago K, Yamamoto S. Inventors; JNC Corp, assignee. Liquid crystal medium, optical device and liquid crystal compound. US patent US 10308870 B2. [2019](#) [2014 Dec 4].
- [428] Jiang T, Chu S, Tian H, et al. Inventors; Beijing Bayi Space LCD Materials Technology Co Ltd, assignee. Liquid crystal compound containing dibenzothiophene structure and application thereof. CN patent CN 109206400 A. [2019](#) [2017 Jul 6].
- [429] Jiang Z. Inventor; Beijing Bayi Space LCD Tech Co Ltd, Dongjin Semichem Co Ltd, assignee. Liquid crystal compound containing difluoromethoxy bridge, composition and application thereof. US patent US 10494569 B2. [2019](#) [2015 Jun 1].
- [430] Okumura K, Masukawa T, Kimura K. Inventors; JNC Corp, assignee. Liquid crystal compound having benzopyran skeleton, liquid crystal composition, and liquid crystal display device. US patent US 10428273 B2. [2019](#) [2017 Jul 21].
- [431] Sasada Y, Sawada M. Inventors; JNC Corp, assignee. Liquid crystal compound, liquid crystal composition and liquid crystal display device. US patent US 10208249 B2. [2019](#) [2017 Sep 19].
- [432] Sato S, Hirata K, Kubo T. Inventors; JNC Corp, assignee. Liquid crystal compound having halogenated alkyl, liquid crystal composition, and liquid crystal display element. JP patent JP 2019167547 A. [2019](#) [2019 May 27].
- [433] Takata A. Inventor; JNC Corp, assignee. Liquid crystal compound having polyfluoro-2-butenoxy group, liquid crystal composition and liquid crystal display device. US patent US 10358602 B2. [2019](#) [2017 Jul 14].
- [434] Takata A. Inventor; JNC Corp, assignee. Compounds having dibenzothiophene ring, liquid crystal composition, and liquid crystal display element. WO patent WO 2019/107394 A1. [2019](#) [2018 Nov 28].
- [435] Tanaka H. Inventor; JNC CORP, assignee. Liquid crystal compound having biphenylene, liquid crystal composition and liquid crystal display device. US patent US 10323187 B2. [2019](#) [2017 Sep 28].
- [436] Tian H, Jiang T, Chu S, et al. Inventors; Beijing Bayi Space LCD Materials Technology Co Ltd, assignee. Negative dielectric anisotropy liquid crystal compound, preparation method and application thereof. CN patent CN 109207160 A. [2019](#) [2017 Jul 3].
- [437] Tian H, Jiang T, Chu S, et al. Inventors; Beijing Bayi Space LCD Materials Technology Co Ltd, assignee. Dibenzothiophene-based negative dielectric anisotropic compound, and preparation method and application thereof. CN patent CN 109423296 A. [2019](#) [2017 Aug 24].
- [438] Yano T. Inventor; JNC Corp, assignee. Liquid crystal compound having benzothiophene, liquid crystal composition and liquid crystal display device. US patent US 10308871 B2. [2019](#) [2016 Feb 10].
- [439] 姜祎, 徐虹, 宋小妹, et al., Inventors; 陕西中医药大学, assignee. 一种侧向四氟取代联苯并杂环化合物及其制备方法. CN patent CN 106699710 B. [2019](#) [2016 Dec 12].
- [440] Babcock John A, Siess Iii Charles P, Watts Kevin G. Inventors; Linde AG, assignee. Y-grade NGL fluids for enhanced oil recovery. US patent US 10570332 B2. [2020](#) [2017 Aug 18].
- [441] Cai Z-Y, Luo S-L, Zeng M-Y, et al. Inventors; daily Xianhua Optoelectronics Materials Co Ltd, Yantai Xinghau Chem Tech Co Ltd, assignee. Negative dielectric anisotropy liquid crystal compound and preparation method and application thereof having an appropriate clearing point and an appropriate optical anisotropy. TW patent TW I697547 B. [2020](#) [2019 May 27].
- [442] Chu S, Zhu BO, Gao L, et al. Inventors; Beijing Bayi Space LCD Materials Technology Co Ltd, assignee. Liquid crystal compound, preparation method and application thereof. CN patent CN 111778040 A. [2020](#) [2019 Apr 3].
- [443] Chu S, Zhu BO, Wang Y, et al. Inventors; Beijing Bayi Space LCD Materials Technology Co Ltd, assignee. Liquid crystal compound with negative dielectric anisotropy as well as preparation method and application thereof. CN patent CN 111718726 A. [2020](#) [2019 Mar 21].
- [444] Chu S, Zhu BO, Wang Y, et al. Inventors; Beijing Bayi Space LCD Materials Technology Co Ltd, assignee. Liquid crystal compound and preparation method and application thereof. CN patent CN 111718725 A. [2020](#) [2019 Mar 21].
- [445] Fujimori S, Inventor; JNC Corp, assignee. Liquid crystal compound comprising benzothiazole ring and CF₂O ligand, liquid crystal composition, and liquid crystal display element. WO patent WO 2020/026583. [2020](#) [2019 Jun 4]; p. A1.
- [446] Gao L, Chu S, Tian H, et al. Inventors; Beijing Bayi Space LCD Materials Technology Co Ltd, assignee. Liquid crystal compound, preparation method and application thereof. CN patent CN 111825534 A. [2020](#) [2019 Apr 23].
- [447] Goto M, Fujimori S. Inventors; JNC Corp, assignee. Compound having naphthalene ring, liquid crystal composition and liquid crystal display device. US patent US 10676669 B2. [2020](#) [2017 Mar 24].
- [448] Jiang Z. Inventor; Beijing Bayi Space LCD Tech Co Ltd, Dongjin Semichem Co Ltd, assignee. Liquid crystal compound containing a difluoromethoxy bridge and application thereof. US patent US 10584086 B2. [2020](#) [2015 Jun 1].
- [449] Mori A, Tanaka H. Inventors; JNC Corp, assignee. Compound having fluorodibenzofuran ring, liquid crystal composition and liquid crystal display device. US patent US 10662378 B2. [2020](#) [2018 Mar 12].
- [450] Okumura K. Inventor; JNC Corp, assignee. Liquid crystalline compound, liquid crystal composition and liquid crystal display element. JP patent JP 2020158394 A. [2020](#) [2019 Mar 25].

- [451] Takata A. Inventor; JNC Corp, assignee. Compound having dibenzofuran ring, liquid crystal composition, and liquid crystal display element. US patent US 2020/0032143 A1. [2020](#) [2018 Feb 16].
- [452] Takata A, Sakamoto A. Inventors; JNC Corp, assignee. Liquid crystalline compound having fluorobiphenyl group and negative dielectric anisotropy, liquid crystal composition, and liquid crystal display element. US patent US 10533136 B2. [2020](#) [2018 Sep 10].
- [453] Wang X, Chu S, Wang Y, et al. Inventors; Beijing Bayi Space LCD Materials Technology Co Ltd, assignee. Liquid crystal compound and preparation method and application thereof. CN patent CN 111484475 A. [2020](#) [2019 Jan 28].
- [454] Wang X, Dai X, Wang Y, et al. Inventors; Beijing Bayi Space LCD Materials Technology Co Ltd, assignee. Liquid crystal compound and preparation method and application thereof. CN patent CN 111592890 A. [2020](#) [2019 Feb 20].
- [455] Wang X, Dai X, Wang Y, et al. Inventors; Beijing Bayi Space LCD Materials Technology Co Ltd, assignee. Liquid crystal compound containing dibenzofuran structure and preparation method and application thereof. CN patent CN 111592517 A. [2020](#) [2019 Feb 20].
- [456] Wang X, Dai X, Wang Y, et al. Inventors; Beijing Bayi Space LCD Materials Technology Co Ltd, assignee. Liquid crystal compound and preparation method and application thereof. CN patent CN 111592889 A. [2020](#) [2019 Feb 20].
- [457] Wittek M, Klass D. Inventors; Merck Patent GmbH, assignee. Liquid-crystalline medium, compounds, and high-frequency components. US patent US 10858587 B2. [2020](#) [2017 Oct 18].
- [458] Yano T. Inventor; JNC CORP, assignee. Liquid crystal compound having benzothiophene, liquid crystal composition and liquid crystal display device. US patent US 10563126 B2. [2020](#) [2016 May 10].
- [459] 後藤 泰, 奥村 一. inventors; JNC CORP, assignee. 両端にアルケニルを有する化合物、液晶組成物および液晶表示素子. JP patent JP 6677122 B2. [2020](#) [2016 Aug 9].
- [460] 高田 章. inventor; JNC CORP, assignee. ジフルオロメチレンオキシ基を有する液晶性化合物、液晶組成物および液晶表示素子. JP patent JP 6708042 B2. [2020](#) [2016 Jul 27].
- [461] Dai X, Jiang KUN, Xie PEI, et al. Inventors; Beijing Bayi Space LCD Materials Technology Co Ltd, assignee. Dibenzothiophene sulfone liquid crystal compound as well as preparation method and application thereof. CN patent CN 113684036 A. [2021](#) [2020 May 19].
- [462] Dai X, Su X, Xie PEI, et al. Inventors; Beijing Bayi Space LCD Materials Technology Co Ltd, assignee. Liquid crystal compound containing phenanthrene structure and preparation method and application thereof. CN patent CN 113088292 A. [2021](#) [2020 Jan 8].
- [463] Dai X, Xie PEI, Cheng Y, et al. Inventors; Beijing Bayi Space LCD Materials Technology Co Ltd, assignee. Liquid crystal compound containing cyclohexene structure and preparation method and application thereof. CN patent CN 113265260 A. [2021](#) [2020 Feb 14].
- [464] Deng S, Jiang KUN, Chu S, et al. Inventors; Beijing Bayi Space LCD Materials Technology Co Ltd, assignee. Liquid crystal compound containing dibenzothiophene structure and preparation method and application thereof. CN patent CN 112980459 A. [2021](#) [2019 Dec 13].
- [465] Inagaki J, Kimura K, Takahashi M. Inventors; JNC Corp, assignee. Compound, liquid crystal composition, and liquid crystal display element. JP patent JP 2021187742 A. [2021](#) [2020 May 26].
- [466] Jiang KUN, Deng S, Chu S, et al. Inventors; Beijing Bayi Space LCD Materials Technology Co Ltd, assignee. Bridged-cycloalkane-containing liquid crystal compound as well as preparation method and application thereof. CN patent CN 112980458 A. [2021](#) [2019 Dec 13].
- [467] Jiang KUN, Deng S, Han Y, et al. Inventors; Beijing Bayi Space LCD Tech Co Ltd, assignee. Negative dielectric liquid crystal compound, preparation therefor, and application thereof. WO patent WO 2021/121022 A1. [2021](#) [2020 Dec 1].
- [468] Zhang H, Deng S, Chu S, et al. Inventors; Beijing Bayi Space LCD Tech Co Ltd, assignee. Liquid crystal compound, preparation method therefor and use thereof. WO patent WO 2021/115155 A1. [2021](#) [2020 Dec 1].
- [469] Zhang H, Li H, Li M, et al. Inventors; Shijiazhuang Chengzhi Yonghua Display Materials Co Ltd, assignee. Negative liquid crystal compound, liquid crystal composition, liquid crystal display element, and liquid crystal display. CN patent CN 113354607 A. [2021](#) [2020 Mar 6].
- [470] 松田 智, 田中 裕. inventors; JNC CORP, assignee. フルオレンとCF₂Oを有する液晶性化合物、液晶組成物及び液晶表示素子. JP patent JP 6919394 B2. [2021](#) [2017 Aug 1].
- [471] 澤田 道. inventor; JNC CORP, assignee. ジベンズチオフェン環を有する化合物、液晶組成物、および液晶表示素子. JP patent JP 6939241 B2. [2021](#) [2017 Aug 18].
- [472] 藤森 さ. inventor; JNC CORP, assignee. ベンズチアゾール環とCF₂O結合基とを有する液晶性化合物、液晶組成物、および液晶表示素子. Patent JP WO2020026583 A1. [2021](#) [2019 Jun 4].
- [473] Bremer M, Haas H, Fortte R, et al. Inventors; Merck Patent GmbH, assignee. Liquid-crystalline compounds. WO patent WO 2022/175219 A1. [2022](#) [2022 Feb 15].
- [474] Bremer M, Manabe A. Inventors; Merck Patent GmbH, assignee. Cyanopyrimidine derivatives. US patent US 11261163 B2. [2022](#) [2017 Mar 22].
- [475] Brocke C, Klass D, Fritzsche C. Inventors; Merck Patent GmbH, assignee. Aromatic isothiocyanates. WO patent WO 2022/090099 A1. [2022](#) [2021 Oct 25].
- [476] Dai X, Jiang KUN, Liu D, et al. Inventors; Beijing Bayi Space LCD Tech Co Ltd, assignee. Liquid crystal compound containing cyclohexene structure, preparation method therefor and use thereof. WO patent WO 2022/105790 A1. [2022](#) [2021 Nov 17].
- [477] Dai X, Jiang KUN, Tang Y, et al. Inventors; Beijing Bayi Space LCD Tech Co Ltd, assignee. Liquid crystal compound and method for preparation thereof and application thereof. WO patent WO 2022/116826 A1. [2022](#) [2021 Nov 17].
- [478] Feng J, Zhang H, Sun J, et al. Inventors; Beijing 8 Billion Space Time Liquid Crystal Science and Tech Limited

- Company, assignee. Negative liquid crystal compound as well as preparation method and application thereof. CN patent CN 114105940 A. [2022](#) [2020 Aug 27].
- [479] Huang Y, Qiao Y, Wen G, et al. Inventors; Shijiazhuang Chengzhi Yonghua Display Materials Co Ltd, assignee. Positive dielectric anisotropic liquid crystal composition and liquid crystal display device. US patent US 11466214 B2. [2022](#) [2019 Apr 29].
- [480] Inagaki J, Kimura K, Takahashi M, et al. Inventors; JNC Corp, Chisso Petrochemical Corp, Sagami Chem Res Inst, assignee. Compound, liquid crystal composition, and liquid crystal display element. CN patent CN 114787130 A. [2022](#) [2021 Mar 24].
- [481] Jiang W, Dai X, Tang Y, et al. Inventors; Beijing 8 Billion Space Time Liquid Crystal Science and Tech Limited Company, assignee. Liquid crystal compound and preparation method and application thereof. CN patent CN 114105966 A. [2022](#) [2020 Aug 26].
- [482] Li J, Mo L, Wan D, et al. Inventors; Xian Modern Chemistry Res Inst, Xian Colored Crystal Photoelectric Science and Tech Co Ltd, assignee. Negative dielectric anisotropy liquid crystal compound, composition and display element. CN patent CN 114262323 A. [2022](#) [2021 Nov 24].
- [483] Zhu BO, Dai X, Bian KUN, et al. Inventors; Beijing Bayi Space LCD Tech Co Ltd, assignee. Thiophene-containing liquid crystal compound, preparation method therefor and use thereof. WO patent WO 2022/068499 A1. [2022](#) [2021 Aug 30].
- [484] 姜坤, 邓师勇, 储士红, et al. inventors; 北京八亿时空液晶科技股份有限公司, assignee. 一种含桥环烷烃液晶化合物及其制备方法与应用. CN patent CN 112980458 B. [2022](#) [2019 Dec 13].
- [485] 後藤 泰, 奥村 一, 高田 章, et al. inventors; J N C 株式会社 J N C 石油化学株式会社, assignee. 液晶性化合物、液晶組成物および液晶表示素子. JP patent JP 7187819 B2. [2022](#) [2018 May 22].
- [486] 戴雄, 姜坤, 谢佩, et al. inventors; 北京八亿时空液晶科技股份有限公司, assignee. 一种二苯并噻吩砜液晶化合物及其制备方法和应用. CN patent CN 113684036 B. [2022](#) [2020 May 19].
- [487] 戴雄, 谢佩, 程友文, et al. inventors; 北京八亿时空液晶科技股份有限公司, assignee. 一种含环己烯结构的液晶化合物及其制备方法与应用. CN patent CN 113265260 B. [2022](#) [2020 Feb 14].
- [488] Aihara H, Hayashi K, Watanabe M, et al. inventors; JNC CORP. Chisso Petrochemical Corp, Sagami Chem Res Inst, assignee. Compound, liquid crystal composition, and liquid crystal display element. CN patent CN 117263781 A. [2023](#) [2023 Jun 15].
- [489] Laut Sven C, Brocke C, Manabe A, et al. Inventors; Merck Patent GmbH, assignee. Liquid crystalline medium. WO patent WO 2023/180505 A1. [2023](#) [2023 Mar 24].
- [490] Liu Y, Du W, Gao AA, et al. Inventors; Xian Caijing Opto Electrical Science & Tech Co Ltd, assignee. Preparation method of tetrahydropyran ring negative liquid crystal monomer. CN patent CN 116283869 A. [2023](#) [2023 Feb 17].
- [491] Sun C, Yang Y, Zhao T, et al. Inventors; Jiangsu Hecheng Display Tech, assignee. Liquid crystal composition and liquid crystal display device comprising the same. US patent US 11788010 B2. [2023](#) [2022 Oct 26].
- [492] Brocke C, Taugerbeck A, Klass D, et al. Inventors; Merck Patent GmbH, assignee. Liquid crystal medium. WO patent WO 2024/260902 A1. [2024](#) [2024 Jun 17].
- [493] Tian H, Guo W, Li L, et al. Inventors; Beijing Bayi Space LCD Tech Co Ltd, assignee. Alkenyl group-containing liquid crystal compound, preparation method therefor and use thereof. WO patent WO 2024/160279 A1. [2024](#) [2024 Feb 2].
- [494] Tian H, Jiang KUN, Liu D, et al. Inventors; Beijing Bayi Space LCD Tech Co Ltd, assignee. Dibenzothiophene liquid crystal compound, and preparation method therefor and use thereof. WO patent WO 2024/120149 A1. [2024](#) [2023 Nov 16].
- [495] Tian H, Zhang H, Tang WEI, et al. Inventors; Beijing Bayi Space LCD Materials Technology Co Ltd, assignee. Liquid crystal compound and preparation method and application thereof. CN patent CN 118344880 A. [2024](#) [2023 Jan 13].
- [496] Wu S, Li B, Yuan Q, et al. Inventors; Univ Wuhan Polytechnic, assignee. DI-(+/-)-beta-methyl amyl terphenyl liquid crystal compound as well as preparation method and application thereof. CN patent CN 117510315 A. [2024](#) [2023 Nov 8].
- [497] Wu S, Yuan Q, Lei M, et al. Inventors; Univ Wuhan Polytechnic, assignee. Isothiocyano trans-cyclohexyl biphenyl liquid crystal composition and application thereof. CN patent CN 117903814 A. [2024](#) [2023 Nov 9].
- [498] Brocke C, Klass D, Jost M, et al. Inventors; Merck Patent GmbH, assignee. Liquid crystal medium. US patent US 2025/0154412 A1. [2025](#) [2024 Oct 29].
- [499] Brocke C, Klass D, Jost M, et al. Inventors; Merck Patent GmbH, assignee. Indene derivatives. WO patent WO 2025/196107 A1. [2025](#) [2025 Mar 19].
- [500] Ding W, Wang P, Yang Y, et al. Inventors; Jiangsu Hecheng Display Tech, assignee. Liquid crystal compound, liquid crystal composition thereof, and liquid crystal display device. US patent US 2025/0171690 A1. [2025](#) [2022 Sep 26].
- [501] Parham Amir H, Brocke C, Fritzsche C, et al. Inventors; Merck Patent GmbH, assignee. Heterocyclic compounds for liquid crystals. US patent US 12241012 B2. [2025](#) [2023 Aug 25].
- [502] Wang J, Lee H-K, Laut Sven C, et al. Inventors; Merck Patent GmbH, assignee. Liquid crystal medium. US patent US 2025/0361444 A1. [2025](#) [2025 Apr 28].
- [503] 吴胜莉, 袁骞, 雷孟龙, et al. Inventors; 武汉轻工大学, assignee. 异硫氰基反式环己基联苯类液晶组合物及其应用. CN patent CN 117903814 B. [2025](#) [2023 Nov 9].
- [504] Landrum G. RDKit: open-source cheminformatics. [2006](#).
- [505] Wang S, Witek J, Landrum GA, et al. Improving conformer generation for small rings and macrocycles based on distance geometry and experimental torsional-angle preferences. J Chem Inf Model. [2020](#);60(4):2044–2058. doi: [10.1021/acs.jcim.0c00025](#)
- [506] Frisch MJ, Trucks GW, Schlegel HB, et al. Gaussian 16 Rev. C.01. Wallingford CT; [2016](#).

- [507] Grimme S, Hansen A, Ehlert S, et al. R2SCAN-3c: a “Swiss army knife” composite electronic-structure method. *J Chem Phys.* **2021**;154(6):064103. doi: [10.1063/5.0040021](https://doi.org/10.1063/5.0040021)
- [508] Neese F. Software update: the ORCA program system—version 5.0. *WIREs Comput Mol Sci.* **2022**;12(5):e1606. doi: [10.1002/wcms.1606](https://doi.org/10.1002/wcms.1606)
- [509] McInnes L, Healy J, Melville J. Umap: uniform Manifold Approximation and Projection for Dimension Reduction. *arxiv preprint arXiv:180203426.* **2018**.
- [510] Adamczyk J, Ludynia P. Scikit-fingerprints: easy and efficient computation of molecular fingerprints in Python. *SoftwareX.* **2024**;28:101944. doi: [10.1016/j.softx.2024.101944](https://doi.org/10.1016/j.softx.2024.101944)
- [511] Paszke A, Gross S, Massa F, et al. PyTorch: an imperative style, high-performance deep learning library. *Adv Neural Inf Process Syst.* **2019**;32:8024–8035.
- [512] Parton-Barr C, Berrow SR, Gibb CJ, et al. Deep learning directed synthesis of fluid ferroelectric materials. *arxiv preprint arxiv:2512.16671.* **2025**.
- [513] Chen T, Guestrin C. Xgboost: a scalable tree boosting system. *arXiv preprint, arXiv:1603.02754.* **2016**.
- [514] Palacio-Betancur V, Jackson NE. Molecular charge topologies govern polar nematic ordering. *J Am Chem Soc.* **2025**;147(51):46841–46846. doi: [10.1021/jacs.5c18760](https://doi.org/10.1021/jacs.5c18760)
- [515] Kränz H, Vill V, Meyer B. Prediction of material properties from chemical structures. The clearing temperature of nematic liquid crystals derived from their chemical structures by artificial neural networks. *J Chem Inf Comput Sci.* **1996**;36(6):1173–1177. doi: [10.1021/ci960482r](https://doi.org/10.1021/ci960482r)
- [516] Johnson SR, Jurs PC. Prediction of the clearing temperatures of a series of liquid crystals from molecular structure. *Chem Mater.* **1999**;11(4):1007–1023. doi: [10.1021/cm980674x](https://doi.org/10.1021/cm980674x)
- [517] Antanasijević D, Antanasijević J, Pocajt V, et al. A GMDH-type neural network with multi-filter feature selection for the prediction of transition temperatures of bent-core liquid crystals. *RSC Adv.* **2016**;6(102):99676–99684. doi: [10.1039/C6RA15056J](https://doi.org/10.1039/C6RA15056J)
- [518] Le TC, Conn CE, Burden FR, et al. Computational modeling and prediction of the complex time-dependent phase behavior of lyotropic liquid crystals under in meso crystallization conditions. *Cryst Growth Des.* **2013**;13(3):1267–1276. doi: [10.1021/cg301730z](https://doi.org/10.1021/cg301730z)
- [519] Sigaki HY, de Souza RF, de Souza RT, et al. Estimating physical properties from liquid crystal textures via machine learning and complexity-entropy methods. *Phys Rev E.* **2019**;99(1):013311. doi: [10.1103/PhysRevE.99.013311](https://doi.org/10.1103/PhysRevE.99.013311)
- [520] Pessa AAB, Zola RS, Perc M, et al. Determining liquid crystal properties with ordinal networks and machine learning. *Chaos, Solitons Fractals.* **2022**;154:111607. doi: [10.1016/j.chaos.2021.111607](https://doi.org/10.1016/j.chaos.2021.111607)
- [521] Zhou Z, Joshi C, Liu R, et al. Machine learning forecasting of active nematics. *Soft Matter.* **2021**;17(3):738–747. doi: [10.1039/D0SM01316A](https://doi.org/10.1039/D0SM01316A)
- [522] Mantel C, Sogaard J, Bech S, et al. Modeling the quality of videos displayed with local dimming backlight at different peak white and ambient light levels. *IEEE Trans Image Process.* **2016**;25(8):3751–3761. doi: [10.1109/TIP.2016.2576399](https://doi.org/10.1109/TIP.2016.2576399)