Contribution ID : **166** Type : **Poster Presentation**

The Structure of the Ferroelectric Nematic Phase: Insights from Molecular Dynamics Simulations

The reported experimental discovery of a ferroelectric nematic (NF) phase is an exciting new development in liquid crystal research. [1-3] The new phase has several potential applications in displays and novel technology due to its unprecedented polarization. However, the origins of the phase are poorly understood, leading to derivatives of the first two mesogens to be discovered, making up most of the known NF mesogens.[1] At a molecular level, the phase is unusual, as often molecules with large dipole moments preferentially align with anti-parallel dipole ordering, as seen (for example) in cyanobiphenyl-based nematics, such as 5CB. However, in the NF phase, large molecular dipoles preferentially align in a parallel direction. [4]

Here, we report state-of-the-art atomistic molecular dynamics simulations of an NF mesogen: "DIO-F" (Fig. 1). We initially use quantum chemical calculations to optimise a new force field for DIO-F, and from molecular dynamics simulations of up to 648 molecules, we obtain excellent predictions of phase properties and transition temperatures. The NF phase is obtained by cooling an isotropic phase and allowing the NF phase to grow slowly over hundreds of nanoseconds of simulation. Cylindrical distribution functions are calculated to investigate the role of specific preferred intermolecular pairings. The calculations allow different explanations for the stability of the NF phase to be probed. NF stability is found to be promoted by a combination of local quadrupolar interactions and microphase separation of hydrophobic parts of the molecule. These interactions are sufficient to overcome the tendency for anti-parallel dipole alignment that is seen in many low molecular weight nematic and smectic systems.

Figure 1: Visualization of a ferroelectric nematic phase of "DIO-F ".

[1] R. J. Mandle; Soft Matter 2022, 18, 5014. [2] X. Chen, et al., Proc. Natl. Acad. Sci. U.S.A. 2020, 117, 14021. [3] R. J. Mandle et al., Nat. Commun. 2021, 12, 4962. [4] M. Mello; M. R. Wilson; T. Araki; Soft Matter 2025, 21, 1479-1488.

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