Physical origin of forming ferroelectric nematic phase

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The nematic phase is a distinct state among liquid crystal phases, characterized by the alignment of rod-like molecules along a preferred direction. In the ordinary nematic phase, the preservation of head-tail symmetry prevents the manifestation of ferroelectricity, which has been not discovered for a long time. It was not until 2017 that the experimental realization of two distinct low molecular weight compounds exhibiting ferroelectricity marked a significant breakthrough. Despite extensive studies, the physical mechanism underlying the emergence of ferroelectricity in nematic liquid crystals remains elusive. This study aims to explore and understand the unique properties and underlying mechanisms of this phase.

Our investigation focuses on systems composed of DIO. Utilizing Gaussian16, we obtained the electric charge distribution to assign the partial charge on each atom. Subsequently, employing GROMACS, we conducted molecular dynamics simulations of 1000 DIO molecules. To elucidate the roles of electrostatic interaction, we also carried out simulations of 2048 DIO molecules without the electric charges.

Our simulations reveal spontaneous polarization in the charged DIO, albeit with the polarization degree smaller than the experimental observations. We attribute this weaker ferroelectricity to computational limitations, as molecular motions are quite slow within the simulation time. On the other hand, spontaneous polarization is not observed in the chargeless system, indicating the electrostatic interaction promotes polarization, in contrast to ordinary nematic phases.

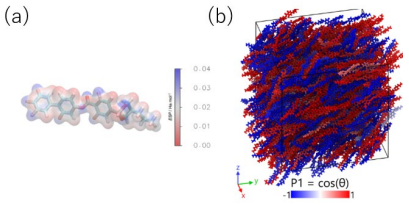

Fig. 1: (a) Electrostatic isopotential of DIO. (b) Snapshot of the DIO system at 330K.

References

[1] H. Nishikawa, *et al*., Adv. Matter. **29**, 1702354 (2017).[2] R. J. Mandle, *et al*., Phys. Chem. Chem. Phys. **19**, 11429 (2017).