Orientational order and molecular dynamics in the polar nematic structures. Electro-optic and elastic properties.

The term liquid crystals (LCs) refers to the state of matter, intermediate between an isotropic liquid and a solid, with properties in between. The liquid crystal state is unique and there is a rich variety of phases in which a given material may exhibit one or more. The least ordered of these phases is the nematic phase, in which the components show long-range orientation order but no long- range translational order. A simple uniaxial nematic phase (N) formed by non-chiral molecules is the most widely studied and technologically exploited of the liquid crystalline phases. On the other hand, it is known that chiral molecules form a twisted (chiral) nematic phase (N*) and three so-called "blue" phases characterized by a lattice of line defects. Only in the last decade have new nematic phases added to this list. In 2011, a spatially modulated twist-bend (N_{TB}) nematic phase was discovered for non-chiral flexible dimer (banana-like) molecules. The long range helical orientation order appears on the 10 nm scale and is a unique example in the nature of the spontaneous mirror symmetry breaking. The helicoid period is in nanoscale range, and therefore the expected electro-optical response time is extremely short of about 1μs as compare to ms range for conventional nematic materials. Then the splay-bend nematic (N_{SB}) was discovered in banana-like colloids and in an electric field applied to the N_{TB} phase. This phase can be characterized as a linearly polarized periodic wave of alternating splay and bend deformations of the averaged orientation order. The N_{SB} phase, in contrast to the N_{TB}, is non-chiral and globally biaxial. As part of the OPUS 2018/31 /B /ST3/03609 grant (end date: 2022-30-06), we successfully studied these structures, and the most important results explaining their self-organization and electro-optical properties were published in seven articles. The greatest achievement was the observation of the phase structure change as a result of surface effects and the electric field. The field-induced distortional effect in the N_{TB} may be extremely useful for technological applications as this has similarity to the electro-clinic effect similar as observed in smectic phases (PCCP 2019, 21, 22839). In the last two years, thermotropic polar nematic phases have been experimentally discovered. An anti-ferroelectric splay nematic (N_S) and a ferroelectric nematic (N_F) for wedge-shaped (pear-like) mesogens with large electric dipole moment (~ 11 D for RM734) have been found. The idea that the nematic phase could be ferroelectric was first proposed by Born in 1916. Despite the fact that the idea was simple, its implementation turned out to be very difficult, the dipole interactions are too weak and the thermal moves in the liquid too strong to obtain a long-range ordering of the dipole moments. Until now, the polar order in the liquid crystal phases is a side effect of steric interactions, and not a direct result of electric dipole interactions. Polar ordering can be achieved by lowering the phase symmetry due to molecular chirality or by strongly inhibited rotation forced by the shape of the molecule, e.g. by bending the core. The recently discovered NF phase and its polar order may also be due to the specific shape of the molecules. In these materials, the observed ferroelectric switching is on the order of 10-100 μs, which is significantly longer than that observed in the twist-bend phases. Nevertheless, the materials that make up the N_{TB}, N_{SB}, N_S and N_F phases are polar materials and have great potential to change the face of future technologies (e.g. as parts of ultra-fast, energy-saving displays, flexible memory, supercapacitors).

The main goal of the project will be to determine the relationship between the molecular structure and the resulting macroscopic properties of the material creating nematic polar phases. To achieve this, it is necessary to determine the orientation and polar order for a group of liquid crystals (LC) with a different molecular structure as well as for mixtures of compounds with different molecular shapes. The proposed research plan includes the synthesis of new materials suspected of forming a nematic polar phase as well as an attempt to produce mixtures of the N_{TB} and N_F materials in order to produce a polar structure with three-dimensional arrangement of molecules. Experimental research will be combined with modeling of DFT under periodic conditions that will allow to predict the stability and properties of polar phases. Using polarization microscopy, infrared and Raman spectroscopy, measurements of the refractive index anisotropy and dielectric permittivity anisotropy, the transition temperatures of the respective mesophases and the appropriate anisotropy values will be determined.