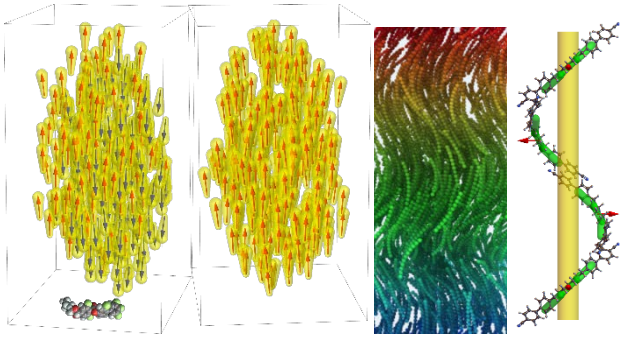

Snapshots of molecular organization in two of recently discovered nematics (left to right): reference uniaxial nematic of strongly polar RM734 molecule (bottom); (hypothetical) ferroelectric nematic phase of RM734; nematic twist-bend (N_{TB}); details of molecular arrangement of CB7CB molecules in N_{TB}. Arrows represent molecular dipole moments.

Nematic liquid crystals are orientationally ordered anisotropic liquids without long-range translational order. Molecular centers of mass are distributed randomly imparting fluidity to these phases, but orientational order is of long range character. Until very recently only two families of nematics were recognized: (1) uniaxial (N_U) and biaxial nematics for nonchiral liquid crystalline materials and (2) cholesteric phase and blue phases for chiral liquid crystals. One of the most spectacular recent discovery is the identification of new nematics (NN) with polar superstructures, belonging to the first family. It started with the discovery of chiral heliconical N_{TB} phase for achiral (banana-like) mesogens, in 2011. The long-range heliconical orientational order of N_{TB}, with pitch on the 10-nm scale, emerges from the N_U phase. It represents a unique in nature example of spontaneous mirror symmetry breaking with no support from any (quasi-)long-range translational order. Then, the nematic splay-bend (N_{SB}) phase has been discovered in bent-shape colloids and under an electric field applied to N_{TB}. It can be characterized as a periodic (linearly polarized wave) of alternating splay- and bend deformations of the average orientational order. But, contrary to N_{TB}, the N_{SB} phase is achiral and globally biaxial.

We studied these structures with success within OPUS 2013/11/B/ST3/04247 (end date: 2018-01-07) with the most important results clarifying their selforganization being published in PNAS, JPCC, Soft Matter and PRE Rapid Communication. But quite recently (i.e. within the last 2 years) experimental groups from EU and the USA have reported further pioneering discoveries. They found an antiferroelectric nematic splay (N_S) and ferroelectric nematic (N_F) for wedge-shaped mesogens with large electric dipole moment (~11 D for RM734), and low-symmetry monoclinic nematic in hybrid materials of disc-like colloids and ordinary nematic liquid crystal. Given that N_{TB}, N_{SB}, N_S and especially N_F are all soft polar materials they have a potential power to change face of future technology (e.g. as being parts of superfast energy-saving flexible displays, flexible memories, supercapacitors etc.). Consequently, NNs have become an extremely "hot" research topic, involving leading groups from the USA, EU, Japan, and China. As the polar and generally orientational selforganization in NNs is poorly understood (perhaps with the exception of N_{TB}) the general aspect of this research proposal is to join this effort and elaborate mesoscopic and microscopic models that will be able to correlate experimental observations (present and future) with relevant molecular features, local symmetry and macroscopic analysis.

Current experiments suggest that the stabilization of NNs can be linked with the observed strong softening of one of the three Frank elastic constants in the parent N_U phase, near the transition to a polar nematic. This, in turn, seems to depend on the molecules' shape through packing entropy and dipolar correlations. Our goal is to explore this hypothesis thoroughly. In particular, we would like to understand why molecules with strong dipole moments, like RM734, prefer ferroelectric arrangement in a 3D liquid state over the energetically more favorable antiparallel, short-range correlations.

Models will be developed to identify the unique molecular structure features responsible for the stabilization of the N_F, N_S and the related phases. Then, with Local Density Functional formalism, generalized deGennes Ginzburg-Landau theory and computer simulations, the theoretical phase diagrams and corresponding phase transitions will be determined. The properties of the novel phases will be predicted and characterized in terms of relevant order parameters. These studies, especially the temperature and electric field dependence of polarization can hint the possibilities for new technological applications. Especially important to the project will be computer simulations (Monte-Carlo, Molecular Dynamic). They will give valuable information about molecular correlations, order parameters, diffusion etc. in the polar nematic phases and, as we hope, shed new light on the nature of the polarity–shape interplay. We should add that the need for models and basic understanding is not just of theoretical interest, but indeed a key requirement for being able to access and further develop the true potential of these materials.