Project A1: Self-assembly of switchable liquid crystal phases at patterned substrates

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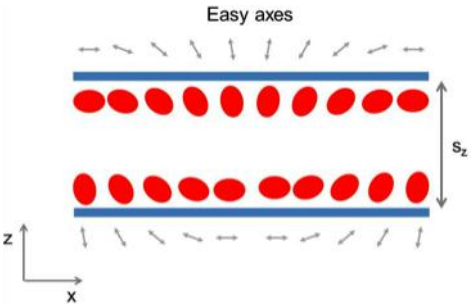
US partners: **Hall (NCSU), Lopez (DU)**

Outline. If a liquid crystal interacts with a solid surface interesting new structures have to be anticipated that may arise on account of the specific way in which molecules are anchored at the substrate surface. By using novel techniques one can nowadays endow planar solid surfaces with specific patterns on a mesoscopic length scale. In this project we consider surfaces separated by a distance s_z along the *z*-axis at which anchoring conditions vary along the orthogonal *x*-direction between homeotropic and planar in a wave-like fashion. We focus on thermodynamic conditions such that the liquid crystal is in its nematic or a smectic phase and investigate the impact of the periodically varying anchoring conditions on the tendency to form orientational and/or positional long-range order. We will consider periodically varying anchoring conditions where the periodicity is different at the two substrates. In addition, anchoring may be out of phase at the two substrates (see figure) such that frustration may arise if the self-assembled structures grow into the third dimension normal to the substrate plane.



Cartoon of confined liquid crystal. Anchoring conditions (easy axes) at the substrates vary periodically along the x-direction. Easy axes may be out of phase (shown); the period of variation may differ between the two substrates (not shown).

Research within the German group. The doctoral researcher working on this project will perform isothermal-isobaric Monte Carlo (MC) and nonequilibrium molecular dynamics (NEMD) simulations where the interactions between a pair of liquid crystal molecules is modeled by a simple anisometric Lennard-Jones potential recently intensively studied by us in the bulk. The fluid-substrate potential consists of a short-range repulsive and an attractive Yukawa-like part which allows us to vary the range of the fluid-substrate interaction while maintaining location and depth of the attractive well. In MC simulations we shall investigate the stability of substrate induced patterns as functions of pattern periodicity and s_z. In addition, a slight modification of the model potential causes molecules to become amphiphilic in nature. We will then focus on the formation of polar phases and their stability to substrate gradients.

Longer-term perspective. Later in the continuation period we will investigate relaxation phenomena in NEMD simulations that arise when the anchoring conditions are changed according to some time-dependent protocol. In this switching process it will be studied how structural changes can be imprinted on more bulk-like regions of the confined liquid crystal and how formation and stability of these structures depend on the protocol.

Complementary work in US partner group. The previously described studies will be amended by employing liquid-crystal model fluids composed of flexible molecules with which Hall's group has considerable experience. In addition, chiral molecules may be considered. Chirality has been introduced already for the well-known Gay-Berne model. From the interaction with Lopez the development of experimentally more realistic surfaces is envisioned.

Status of the project. The project will interact closely with project A2 (v. Klitzing) where substrate gradients are realized via grafted polymer brushes. With project A3 (Stark) the present one shares the idea of inducing new phases through switching by applied external fields. Project A4 (Riegler) focuses on two-dimensional aggregates of anisometric organic molecules where the molecular shape is very similar to that of molecules to be studied here. In project C5 (Klapp) the interaction between molecules is of an amphiphilic "Janus"-like nature similar to what will be investigated here. Likewise, anisometric organic molecules are also employed in project C1 (Rabe).