Project C5: Field-driven self-assembly and transport of Janus particles at interfaces

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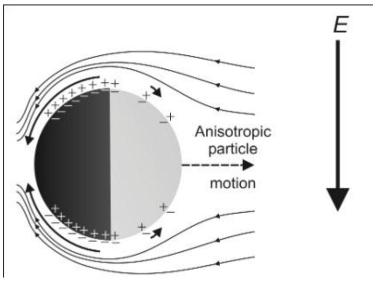
US partners: Velev, Hall (NCSU)

Outline. Recent research has shown that self-assembly and autonomous organization into mesostructures can be found not only in many "passive" systems like colloidal crystals, lipid bi-layers, etc., but also in "active" systems such as bacteria colonies and suspensions of artificial „self-propelling" particles. An example of the latter class are metallodielectric ("Janus") colloids, where nontrivial directed motion can be generated by application of oscillating electric fields (see figure). The present project aims to develop a theoretical understanding of the self-assembly and transport of such Janus particles, which are also a focus of current interest in the experimental group of O. D. Velev (NCSU). From a theoretical perspective, a profound understanding of self-propelling colloids, which are intrinsically out of equilibrium, is just beginning to emerge. In the present project we investigate the *collective* behavior of such particles in a two-dimensional (2D) set-up by particle-based computer simulations, particularly overdamped Brownian Dynamics (BD). We aim to reveal the emergence of typical "active-particle" behavior such as clustering and swarming, and its interplay with the already complex (Janus-like) "passive" interactions between the nanoparticles. Indeed, so far most simulation studies of interacting active particles have rather focussed on steric (exclusion) interactions alone.



*Sketch of self-propelling metallodielectric particle (from Gangwal et al., Phys. Rev. Lett. **100**, 058302 (2008).*

Research within the German group. The PhD student involved in this project will perform BD computer simulations of an effective (solvent-free) model in 2D (consistent with the experiments). The passive interactions between the metallodielectric particles will be modeled by anisotropic pair potentials reflecting the "Janus"-like and dipolar/quadrupolar nature of these particles. The external field (which induces the particle motion) will enter only implicitly via "activity" terms in the (overdamped) BD equations of motion. One possibility is to include an additional force directed along the unit vector of the particle orientation. The equations further involve frictional as well as random forces. Based on this model we will systematically explore, on one hand, structural properties such as clustering/swarming and its interplay with the self-assembly induced by the passive interactions. On the other hand, we will investigate time-dependent properties such as diffusion and cluster sizes.

Longer-term perspective. As a continuation of the project, we will first improve our model by introducing hydrodynamic interactions between the particles. Based on this step, which will substantially complicate the numerical calculations, we aim develop a deeper understanding of, e.g., the impact of solvent viscosity. Second, we will investigate binary systems and possible sorting mechanisms.

Complementary work in the US partner group. One focus of research in the Velev group involves synthesis and microscopy of metallodielectric particles in 2D. During her/his stay in the US, the German student will adjust the simulations to these ongoing experiments. This will be done together with C. Hall, who is an expert in computer simulations of complex fluids. A collaboration with Velev and Hall (on self-assembling „passive" particles) already exists.

Status of the project. The present project will be related to essentially all theoretical projects focussing on the self-assembly of particles with anisotropic interactions. Indeed, the (angle-dependent) passive interactions used here have similarities with those employed in project A1 (Schoen), A3 (Stark), and B5 (Schoen). In addition the present project plans to collaborate with project A2 (v. Klitzing).