TECHNISCHE UNIVERSITÄT WIEN

DESIGN OF ANISOTROPIC DNA ORIGAMI NANOPARTICLES FOR PROGRAMMED SELF-ASSEMBLY

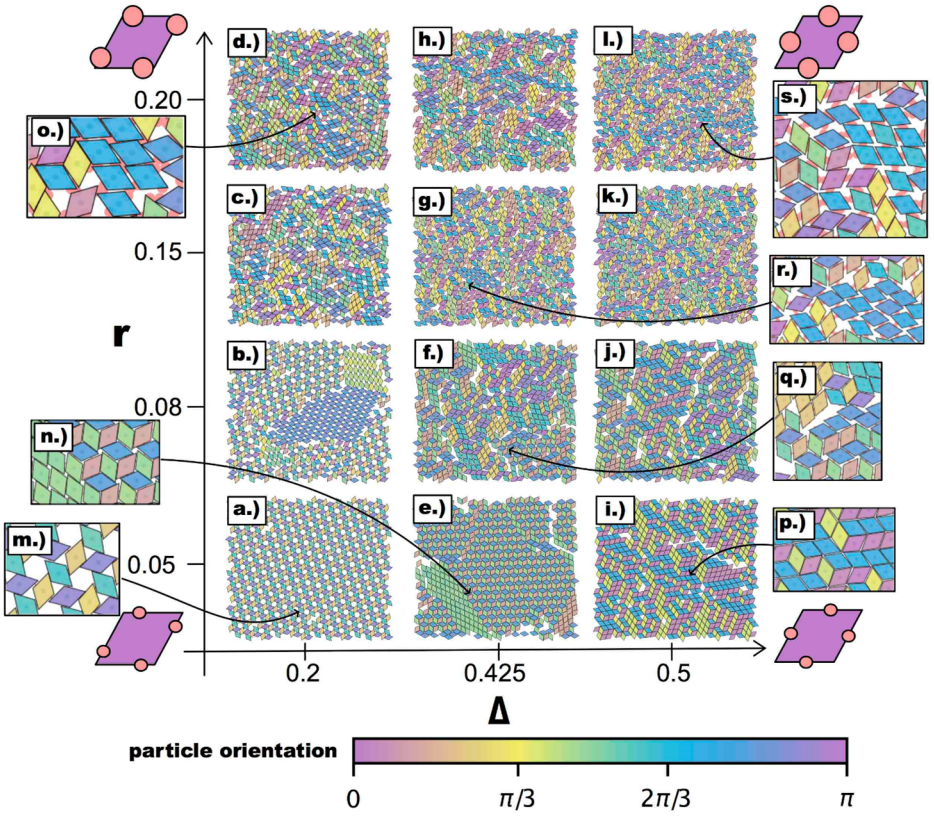

Figure from [1]: Simulation snapshots of the self-assembly products of rhombic platelets with four bonding site placed in the center of each edge for different values of the bonding site position (Δ) and of the bonding site interaction range (r)

Supervisory Team[1]

Primary Supervisor: *Emanuela Bianchi, Soft Matter Group, Institute of Theoretical Physics, TU Wien (Austria)*

TU Wien project partners: *Eva Sevcsik, Biophysics group, Institute of Applied Physics, TU Wien (Austria)*

External academic partners: *Laura Filion, University of Utrecht (The Netherlands)*

Project Description

This PhD project focuses on the self-assembly behavior of functionalized DNA-origami by means of classical many-body simulations of suitably developed coarse-grained models. DNA origami are nowadays emerging as promising nanoparticles with highly tunable interaction

[1]The Early Stage Researchers (ESRs) will be accompanied during their thesis by an individual "Thesis Advisory Committee" (TAC), which will guide the ESR through the graduate studies. The TAC will consist of the thesis primary supervisor, and two additional members of the Supervisory Team selected by the ESR.

properties [2]. They consist of long single stranded DNA molecules that are folded into rigid, two- or three-dimensional shapes by means of connecting shorter staple strands. In addition to the control over their specific shape, DNA-origami can be functionalized, meaning that specific bonding sites can be created by designing a few staple strands to face outwards on specific positions along the DNA-origami surface. The project considers functionalized DNA-origami platelets and aims at developing design rules to guide their self-assembly into two-dimensional structures such as nano-scale carriers and/or porous monolayers for drug delivery, storage or filtering purposes. By means of coarse-grained models and many body simulation approaches, envisioning both classical Monte Carlo and Molecular Dynamic simulations, we will unveil how the DNA-origami building blocks can lead to structures with tailored properties. The proposed work will be directly embedded in the ongoing scientific work of Emanuela Bianchi's group, experimental realizations of functionalized DNA-origami will be synthesized in direct comparison to the simulation results as this project is to be conducted in close collaboration with Eva Sevcsik.

Key Goals and Tasks

The primary aim of this project is to precisely tackle the design principles that govern the self-assembly of functionalized DNA-origami as building blocks of tailored materials. State-of-the-art numerical techniques will be implemented to investigate the collective behavior of suitably developed coarse-grained models of functionalized DNA-origami. Non-spherical hard platelets provided with a small number of bonding sites along their perimeter have been proven to be versatile building units for the assembly of monolayers with a tunable porosity (see the figure) [3]. We will investigate how to optimize the shape and the bonding pattern of such units in order to assemble functional monolayers for technological applications as well as finite clusters that can act as carriers. By efficiently spanning the interaction parameter space, it will be possible to design effective interactions such that they favor specific short- and/or long-range orders. The most challenging part of the proposed project is to deal with the possible kinetic traps of the assembly process; this issue will be tackled by developing molecular dynamics approaches that can reproduce experimentally available tools to trigger the response of the system to external fields.

[1] A Matter of Size and Placement: Varying the Patch Size of Anisotropic Patchy Colloids, C. Karner, F. Müller and E. Bianchi, Int. J. Mol. Sci. 2020, 21, 8621 (2020)

[2] Membrane-Assisted Growth of DNA Origami Nanostructure Arrays, S. Kocabey, S. Kempter, J. List, Y. Xing, W. Bae, D Schiffels, W.M. Shih, F.C. Simmel and T. Liedl, ACS Nano, 9, 3530 (2015)

[3] Design of Patchy Rhombi: From Close-Packed Tilings to Open Lattices, C. Karner, C. Dellago and E. Bianchi, Nano Lett., 19, 7806 (2019)

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Project-specific Requirements

- Completed master studies in Physics, Biophysics, Chemistry and affine fields
- Knowledge on Thermodynamics, Statistical Mechanics and Physical Chemistry
- Experience and skills in programming languages (Fortran, C/C++, Python)
- Interest in developing home-made codes and in the simple modeling of physical systems/phenomena
- Enthusiasm for unveiling the governing principles behind physical phenomena
- Willingness to travel to project meetings and scientific conferences
- Excellent English language skills in scientific field
- Personal skills: curiosity-driven approach, willingness and ability to work in a collaborative team, enthusiasm, good communication skills