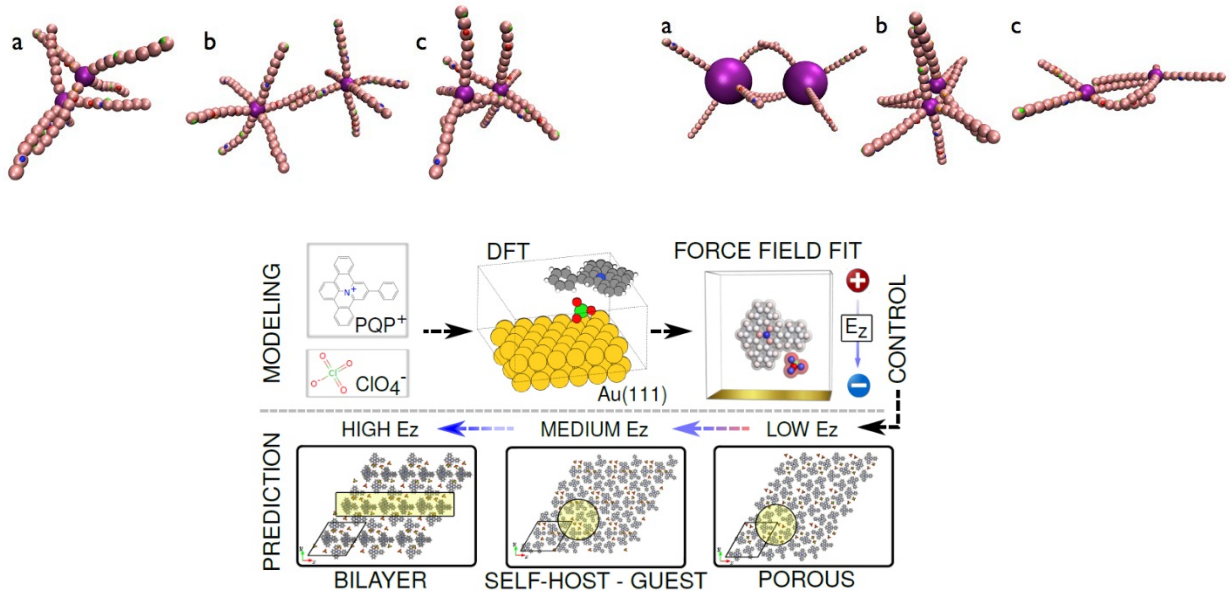
SELF-ASSEMBLY OF BIOLOGICAL, BIO-RELATED AND COLLOIDAL MACROMOLECULES



Top: DNA-coated colloidal particles in various binding configurations.
Bottom: from a model for complex macromolecules to their self-assembly configuration.

Supervisory Team[1]

Primary Supervisor: *Gerhard Kahl, Institute for Theoretical Physics*

TU Wien project partners: *Emanuela Bianchi, Institute for Theoretical Physics, Markus Valtiner, Institute for Applied Physics, Clemens Heitzinger, Institute of Analysis and Scientific Computing, Christian Hellmich, Institute of Mechanics of Materials and Structures*

External academic partners: *Carl Goodrich (IST Austria)*

Project Description

One of the most characteristic features of soft matter and bio-related systems is their propensity to self-assemble into mesoscopic structures. This ability is further supported by the seemingly unlimited freedom to design molecular entities in their synthesis processes with desired shapes and/or target interactions. All these features make such molecules to

[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.

ideal building blocks for self-assembled meso-structures; therefore, soft matter and bio-related systems are considered as promising and versatile systems in the research of functional materials. In an effort to produce particles with desired properties, scientists have to rely on synergetic strategies, reuniting synthesis, experiment, and theory.

The aim of this project is to *predict* with the help of suitable theoretical and numerical tools the possible self-assembly scenarios of experimentally synthesized macromolecular units and to provide hints how these units should be designed in an effort to eventually lead to a desired self-assembly scenario. Particular focus will be put on molecules with aspherical shape which have a considerably higher potential to self-assemble into more exotic structural units. In a subsequent step we plan to investigate the physical properties of these units and to compare them to complementary theoretical concepts and experimental results

The spectrum of our state-of-the-art methods range from theoretical concepts (such as density functional theory) to computer simulations in various ensembles and require heavy computational efforts. In an effort to efficiently scan huge dimensional parameter spaces and to find out common features of obtained structures we rely on artificial intelligence algorithms.

Key Goals and Tasks

The primary aim of this PhD thesis is to help to guide with computer simulations and artificial intelligence algorithms experimentalists to design and to synthesize biological, bio-related and colloidal macromolecules that self-assemble into desired target structures.

Project-specific Requirements

- Completed master studies in Physics or Computational Sciences
- Knowledge on concepts in Theoretical Physics , Computer Simulations, and Artificial Intelligence
- Experience and skills in Computational Sciences
- Enthusiasm, critical thinking, independence, persistence, high proficiency in scientific work
- Readiness to solve problems along unconventional routes
- Readiness to face new challenges and unforeseeable problems
- Readiness to work in different scientific surroundings (stages in other groups, possibly abroad)
- Readiness for interdisciplinary cooperation
- Excellent English language skills
- Ability to work in a team, to contribute to the supervision to younger colleagues