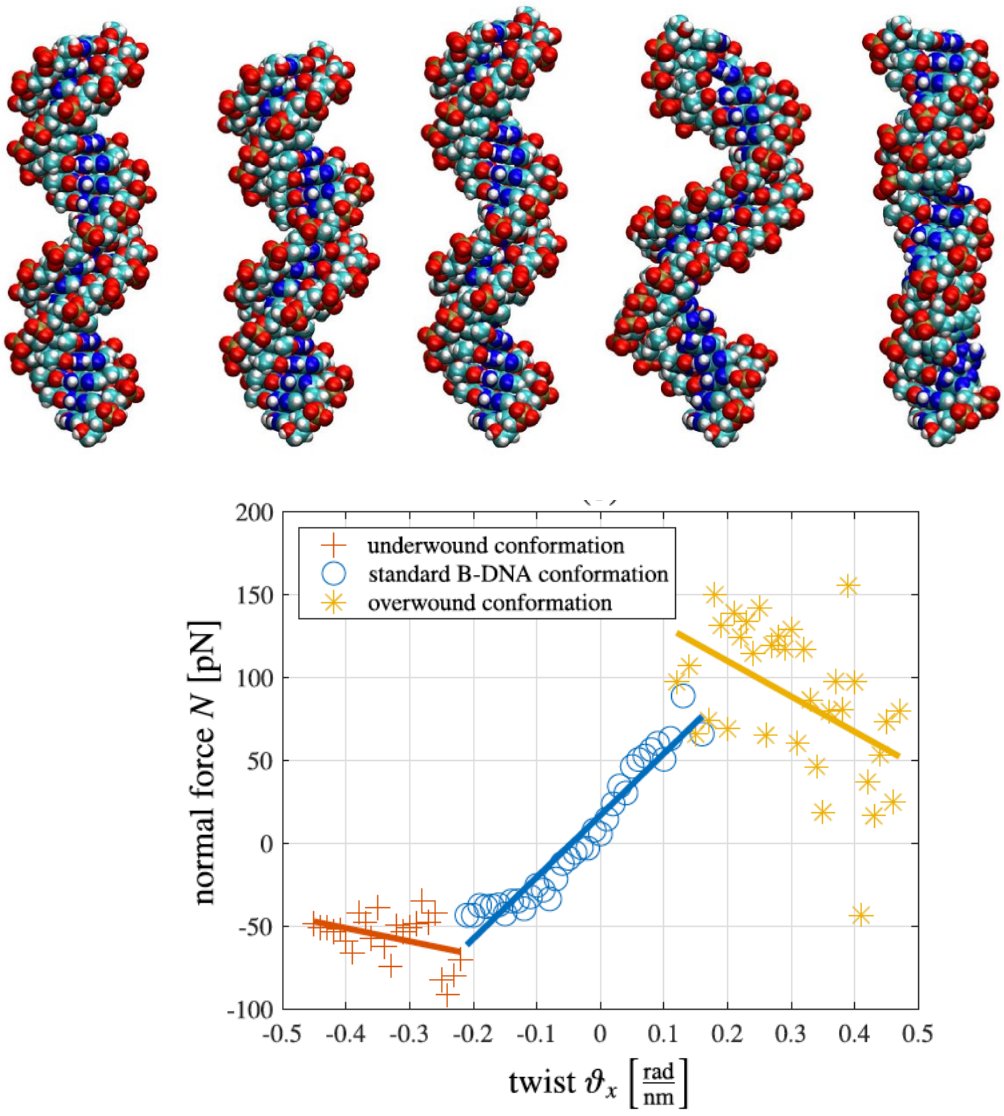
ATOMS-TO-BEAM HOMOGENIZATION OF BIOMACROMOLECULES



Top: Mechanics-driven configurations of B-DNA: loaded, compressed, stretched, overwound, underwound

Bottom: conformation-dependent force-over twist relation

Supervisory Team[1]

Primary Supervisor: *Christian Hellmich, Institute for Mechanics of Materials and Structures*

[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.

TU Wien project partners: *Johannes Kalliauer, Institute for Mechanics of Materials and Structures, Gerhard Kahl, Institute for Theoretical Physics, Gerhard Schütz, Institute for Applied Physics*

External academic partners: *Stéphane Avril (Université de Lyon – Mines Saint-Etienne)*

Project Description

Biomacromolecules fulfill multiple important structural functions in biology, often withstanding significant forces. In fact, it has become increasingly clear that fundamental biological processes such as DNA replication or gene expression come along with essential mechanical deformations of the invokved entities, such as bending, twisting, or stretching of the involved structural entities. However, while atom interaction within the molecules has been mathematically been studied for quite some while, reliable mathematical tools for the simulations of the complex deformation states the sydtems go through are largely missing. As a remedy to this unsatisfying situation, the current project will build on recent work[2], which allowed for linking molecular dynamics with classical structural mechanics, the scientific field covering the deformational behavior of structural components like beams, plates, or shells, by means of the overarching principle of virtual power. This is expected to elucidate and fully quantify the complex coupled deformation behavior of biomacromolecules – which is even conformation-dependent and goes far beyond the often employed linear springs, and their interaction in forming larger intra- or extracellular structures. Thereby, we envision fundamental insights in the newly growing field of mechanobiomics – holding great promises for tackling pressing biological and medical problems, from genetic diseases to COVID-19 healing.

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 Engineering (biomedical, civil, mechanical), Physics, Chemistry, Materials Science or Computational Sciences
- Knowledge on concepts in Engineering Mechanics, Theoretical Physics, and Computer Simulations
- 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

[2] Kalliauer et al, J Mech Phys Sol 143, 104040, 2020

- 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