IMPRS on Multiscale Biosystems

Project description

Title: Modeling molecular interactions of cellulose microfibrils
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In collaboration with: (Luca Bertinetti, John Dunlop)
Project description:
Cellulose, the most abundant natural polymer in nature, packs into dense crystaline microfibrils. Understanding the molecular interaction both within the crystals and of the microfibrils with other polysaccharides, lignin, different proteins, peptide sequences or small molecules is essential for understanding (a) structure and mechanical properties of the plant cell wall, (b) cellulose stability and enzymatic degradation for biofuels and (c) the design of renewable bio-composite materials [1, 2].

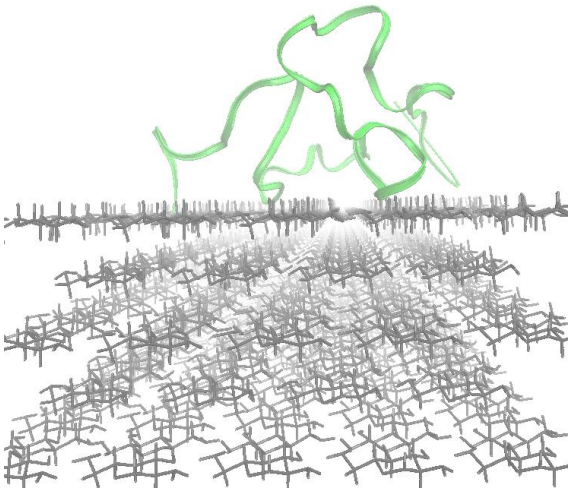

Figure: *Cellulose Fibril interacting with a peptide segment.*

This project aims to understand the effect of the detailed molecular interactions of cellulose on the structure and function at larger scale. The large range of relevant length and timescales in such systems, present a challenge for modeling. The microfibrils reach µm lengths and interact with matrix polymers of 500-1000 sugars, yet details of local structure and interactions play a critical role.

Here, cellulose microfibrils and their interactions with other molecules will be modeled using and combining a variety of computational methods at different scales. The quality of the models prediction will be tested for example by comparison with AFM-based single molecule force spectroscopy measurements.

Required background: Physics, theoretical chemistry, or similar, with background in statistical physics and programming skills. Ideally, the candidate should have experience with molecular simulation methods.
Paper to read before the interview: Beckham, G.T., et al., *Applications of computational science for understanding enzymatic deconstruction of cellulose.* Current Opinion in Biotechnology, 2011. **22**(2): p. 231-238.
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www: www.mpikg.mpg.de/theorie/arbGruppen/multiscaleModelling

References

1. Bellesia, G., et al., Acta Crystallographica Section D-Biological Crystallography, 2011. **66**: p. 1184-1188.
2. Beckham, G.T., et al., Current Opinion in Biotechnology, 2011. **22**(2): p. 231-238.