SUMMARY

1. Research project objective/Hypothesis

This project will investigate the self-assembly and crystallization processes of cellulose microfibrils with different contents of Iα/Iβ allomorphs in the presence of disorder parts, the mechanical characterization via experimental and computational AFM nanoindentation, and the interaction with protein complexes of industrial interest. The aggregates of cellulose microfibrils have several functions in plants and bacteria which span from rigidity of cell-wall and tensile strength to environmental protection. Hence, the proposed research in principle concerns one of the major renewable resources on Earth. The scope of this project will enhance our understanding on the structure of the cellulose and unravel their role during aggregation and crystallization processes.

2. Research project methodology

The aggregation and self-assembly of cellulose microfibril are dictate by a collective behavior and interactions between glucose monomer. Moreover, due to the large time and length scale involved in the description of such processes, computer simulation based on coarse-grained models are well-suited. The theoretical part of the project will be based on Molecular Dynamics simulations of the structure-based model (i.e. Go-like approach) and all-atom force fields. In collaboration with experimentalists Stefan Weber and Horacio Vargas from the Max Planck Institute for Polymer Research, the nanomechanical characterization of cellulose microfibrils will be confirmed by experiment. This methodology is perfectly suitable and transferable for the study of self-assembly process of several biological fibrils such as polyglutamine and β-amyloid fibrils.

3. Research project impact

Understanding the structure-function relationship is of fundamental interested in several disciplines. As it is relevant also in many biological process where the native state of a protein defines a specific function, similarly the coexistence of cellulose Iα/Iβ with disorder parts determines the mechanical function which has great implication in the industrial processes.

The real transition to a more bio-based economy will be only possible via basic research in renewable feedstock. For instance, degradation of cellulose sources like food crops has lead mankind to biofuels, but the process is not yet fully sustainable as it posses serious societal concerns such as the “food vs. fuel”. Agriculture waste and city biomass are among the best cellulosic candidates for biofuel conversion, but yet no an efficient cycle is been designed. A better understanding of cellulose-enzyme interaction can enable the rapid transition to a green economy.