MECHANICAL PROPERTIES OF SINGLE POLYSACCHARIDE, DNA AND PROTEIN MOLECULES STUDIED WITH THE ATOMIC FORCE MICROSCOPE AND COMPUTER SIMULATIONS

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Mechanical properties of biopolymers are of utmost importance in biology. For example, ubiquitous polysaccharides (e.g. cellulose) are the fundamental structural elements of the cell wall in plants and bacteria and in higher organisms they serve as lubricants, provide support to cellular elements of tissues and also participate in numerous molecular recognition and adhesive interactions. Many modular proteins such as titin, fibronectin or spectrin play important roles in regulating molecular elasticity of the structures that they support (muscle, extracellular matrix, cytoskeleton). The mechanical properties of the double helix of DNA critically affect such fundamental processes as transcription, replication, recombination and damage repair.

In this talk I will review my past and most recent research on plastic and elastic deformations of *single* polysaccharides, proteins and DNA which I investigate with the atomic force microscope (AFM). Because AFM can apply significant mechanical forces to these biopolymers it can induce their transitions to new conformations which are typically not sampled in equilibrium. For example, sugar rings of polysaccharides can be forced to acquire high energy boat-like conformations; titin modules can be mechanically unraveled to produce a fully extended conformation of the polypeptide chain and the double helix of DNA can be forced to unwind to a new structure which is extended by ~70 % as compared to the standard B form. Thus, AFM methodologies can provide unique data about biopolymer properties in high energy conformations, which are not accessible to conventional methods of measurements such as NMR spectroscopy and X-ray crystallography. To aid the interpretation of my single-molecule mechanical measurements with the AFM I also model the elastic properties of sugars and proteins using quantum mechanical and molecular dynamics methodologies. These experimental and numerical studies of biopolymers increase our understanding of their functional properties under various mechanical loads and expand the new field of single molecule mechanochemistry.